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GCMS-spor

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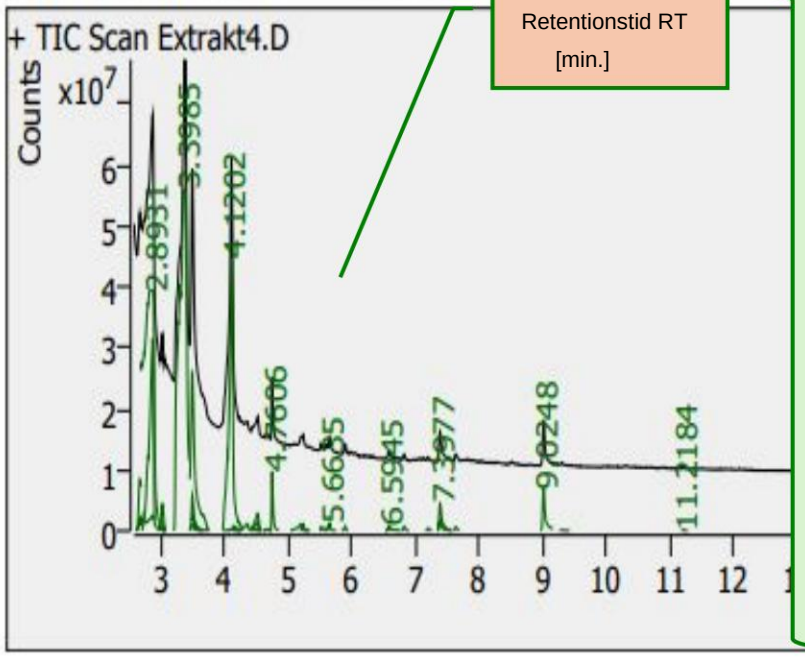
Analyst Name	
Analysis Time	3/27/2024 1:27:01 PM
Data File Name	Extrakt4.D
Sample Name	Extrakt4
Acq Method File	Faserextrakt
Acq Time	3/26/2024 12:52:22 PM
Instrument Name	Intuvo_MSD



Retentionstid RT [min.]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
2.6837	2-Pentanone	107-87-9	C5H10O	19999669		86.6	1.21	4.02
2.6868	Urea, 1-methylcyclopropyl-	58102-14-0	C5H10N2O	6766861		54.5	0.41	1.36
2.7521	2-Propenoic acid, oxiranylmethyl ester	106-90-1	C6H8O3	8001717		63.5	0.49	1.61
2.8842	(Z)-CH3CH2CH=CH(OCH3)	10034-12-5	C5H10O	149191988		74.0	9.05	30.02
2.8879	Oxetane, 3-(1-methylethyl)-	10317-17-6	C6H12O	18991705		57.1	1.15	3.82
2.8931	2,3-Hexanedione	3848-24-6	C6H10O2	461289190		83.7	27.97	92.80
3.0344	2(3H)-Furanone, dihydro-3,5-dimethyl-	5145-01-7	C6H10O2	9524980		86.2	0.58	1.92
3.0590	Carbamic acid, monoammonium salt	1111-78-0	CH6N2O2	1361870		61.4	0.08	0.27
3.3985	Ethanone, 1-cyclopropyl-	765-43-5	C5H8O	497053902		84.9	30.14	100.00
3.5048	Propyl pyruvate	1000431-41-8	C6H10O3	129180976		87.8	7.83	25.99
3.5078	Dimethyl ether	115-10-6	C2H6O	17315014		66.8	1.05	3.48
3.5186	Furan, 2-methoxy-	25414-22-6	C5H6O2	8759503		82.7	0.53	1.76
3.5203	Methanesulfinyl fluoride, trifluoro-	812-12-4	CF4OS	5273045		50.5	0.32	1.06
3.5229	Ethane, 1,1,1-trifluoro-	420-46-2	C2H3F3	1837998		52.1	0.11	0.37
4.1202	2-Pentene, 2,3-dimethyl-	10574-37-5	C7H14	199000520		89.9	12.07	40.04
4.1315	Histamine, N-benzoyl-2-cyano-	74419-68-4	C13H12N4O	1211450		53.5	0.07	0.24
4.1359	1-Pentanone, 1-(2-furanyl)-	3194-17-0	C9H12O2	1019647		59.8	0.06	0.21
4.1580	Water	7732-18-5	H2O	2504771		86.3	0.15	0.50
4.3670	1,5-Dimethyl-1,4-cyclohexadiene	4190-06-1	C8H12	4562178		82.0	0.28	0.92
4.5248	Butanenitrile, 4-(dimethylamino)-	13989-82-7	C6H12N2	161984		61.1	0.01	0.03
4.5320	Cyclohexene, 3,5-dimethyl-	823-17-6	C8H14	12650158		90.8	0.77	2.55
4.5359	Cyclohexene, 4-methyl-	591-47-9	C7H12	6098132		60.2	0.37	1.23
4.5402	N-Benzyloxycarbonyloxy-5-norbornene-2,3-dicarboximide	62210-73-5	C17H15NO5	1328603		50.8	0.08	0.27
4.6697	2-Pentyn-4-one	7299-55-0	C5H6O	637750		68.5	0.04	0.13
4.7036	1,3-Cyclohexadiene, 5,6-dimethyl-	5715-27-5	C8H12	769153		70.8	0.05	0.15
4.7606	Acetone	67-64-1	C3H6O	15824489		95.0	0.96	3.18
5.2109	Benzene, 1,3-dimethyl-	108-38-3	C8H10	4990927		92.9	0.30	1.00
5.2484	(R)-(+)-3-Methylcyclopentanone	6672-30-6	C6H10O	2481356		70.1	0.15	0.50

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
5.5308	(R)-(+)-3-Methylcyclopentanone	6672-30-6	C6H10O	1212191		74.2	0.07	0.24
5.6017	(Z)-3-Heptene	7642-10-6	C7H14	922767		67.0	0.06	0.19
5.6635	Furan, 3-methyl-	930-27-8	C5H6O	2619124		81.2	0.16	0.53
5.9075	1H-Pyrazole, 4,5-dihydro-3-methyl-1-propyl-	26964-49-8	C7H14N2	1382050		75.0	0.08	0.28
6.5887	2-Methylthiolane, S,S-dioxide	1003-46-9	C5H10O2S	617212		73.0	0.04	0.12
6.5945	Cycloheptene	628-92-2	C7H12	3017986		73.2	0.18	0.61
6.8338	Benzene, 1,2,4-trimethyl-	95-63-6	C9H12	1466138		86.2	0.09	0.29
7.2078	N-Methyl methacrylamide	3887-02-3	C5H9NO	794861		68.5	0.05	0.16
7.3954	Ethylbenzene	100-41-4	C8H10	6184923		64.5	0.38	1.24
7.3977	1,3-Hexadiene, 2,5-dimethyl-	29253-64-3	C8H14	14077119		83.6	0.85	2.83
7.4000	1,3,7-Octatriene	1002-35-3	C8H12	4836937		59.8	0.29	0.97
7.5377	1H-Pyrazole-1-carboximidamide, 3,5-dimethyl-	22906-75-8	C6H10N4	475370		64.0	0.03	0.10
7.6467	Cyclohexene, 1,6-dimethyl-	1759-64-4	C8H14	1424397		68.5	0.09	0.29
9.0248	Ethinamate	126-52-3	C9H13NO2	20018408		80.3	1.21	4.03
9.3111	Ethane, 1,2-dibromo-	106-93-4	C2H4Br2	199199		54.3	0.01	0.04
11.2184	Benzene, 1-ethyl-3,5-dimethyl-	934-74-7	C10H14	253850		68.0	0.02	0.05
23.3546	4-Octene, (E)-	14850-23-8	C8H16	1729434		80.7	0.10	0.35

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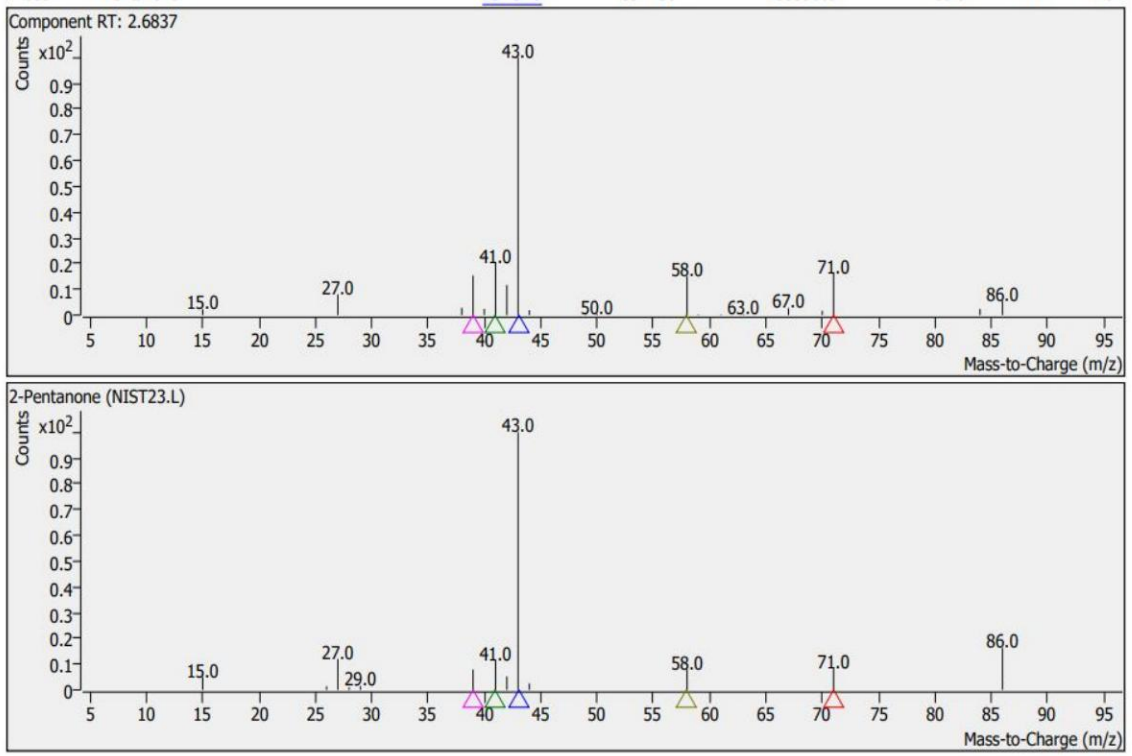
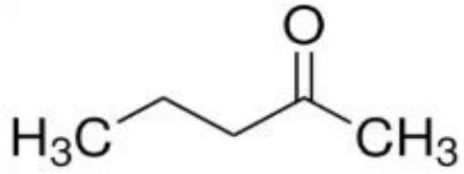
2-Pentanon, CAS 107-87-9 / RT: 2,6837 [ÿ 1,2 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
2.6837	2-Pentanone	107-87-9	C5H10O	19999669		86.6	1.21	4.02





2-Pentanone **Revision Date** 24-Dec-2021

Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Wear protective gloves/protective clothing/eye protection/face protection

Skin

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Fire

In case of fire: Use CO2, dry chemical, or foam for extinction

Storage

Store in a well-ventilated place. Keep cool

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

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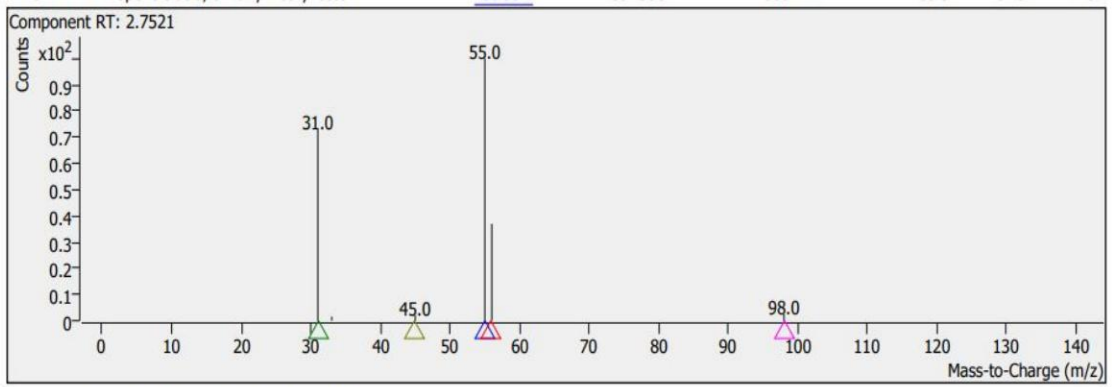
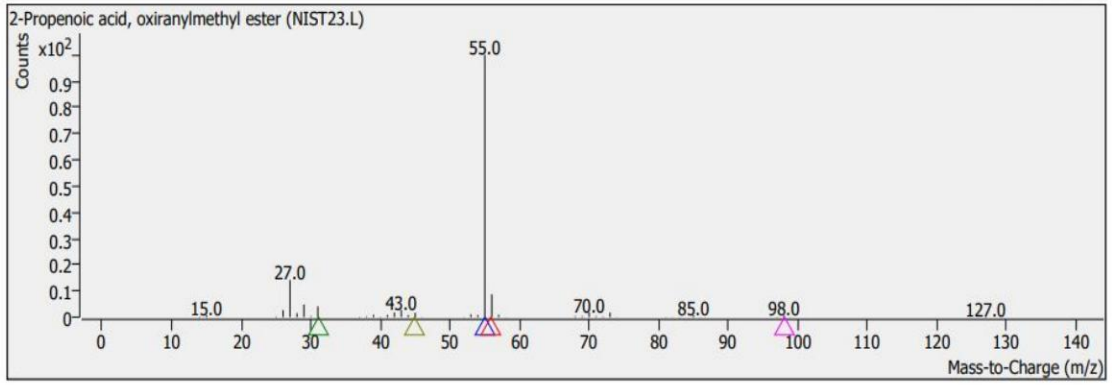
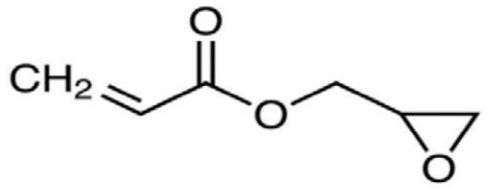
2-Propensyre, oxyranylmethylester, CAS 106-90-1 / RT: 2,7521 [ÿ 0,5 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
2.7521	2-Propenoic acid, oxiranylmethyl ester	106-90-1	C6H8O3	8001717		63.5	0.49	1.61







Danger
H301 Toxic if swallowed
H311 Toxic in contact with skin
H314 Causes severe skin burns and eye damage
H317 May cause an allergic skin reaction
H331 Toxic if inhaled

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P271 Use only outdoors or in a well-ventilated area.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor/...
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P312 Call a POISON CENTER/doctor/...if you feel unwell.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].
P363 Wash contaminated clothing before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P310 Immediately call a POISON CENTER/doctor/...
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
P362+P364 Take off contaminated clothing and wash it before reuse.
P311 Call a POISON CENTER/doctor/...
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P501 Dispose of contents/container to ...

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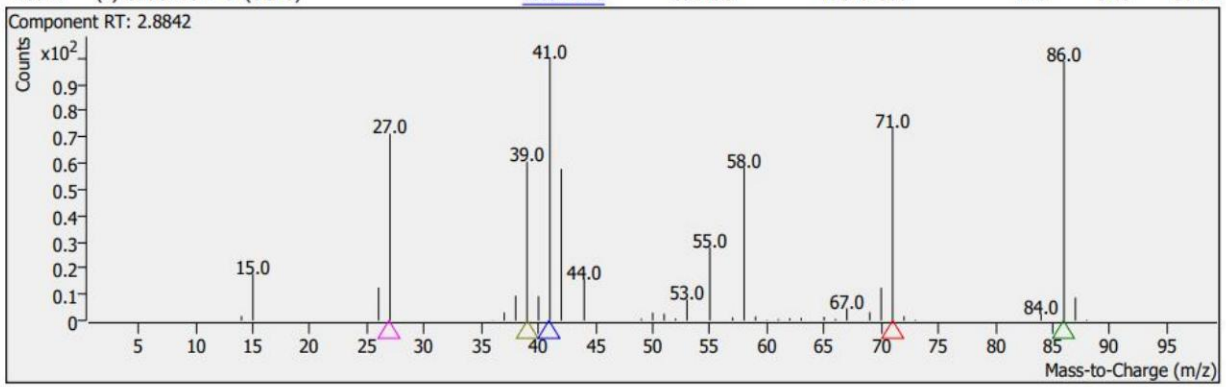
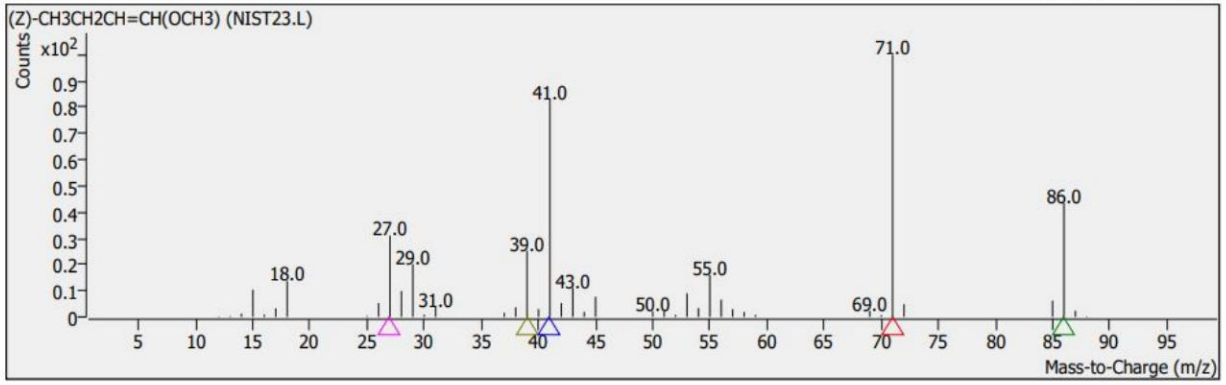
(Z)-CH3CH2CH=CH(OCH3), CAS 10034-12-5 / RT: 2,8842 [ÿ 9,05 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
2.8842	(Z)-CH3CH2CH=CH(OCH3)	10034-12-5	C5H10O	149191988		74.0	9.05	30.02





GHS label elements, including precautionary statements

Pictogram(s)	no data available
Signal word	no data available
Hazard statement(s)	no data available
Precautionary statement(s)	
Prevention	no data available
Response	no data available
Storage	no data available
Disposal	no data available

Other hazards which do not result in classification

no data available

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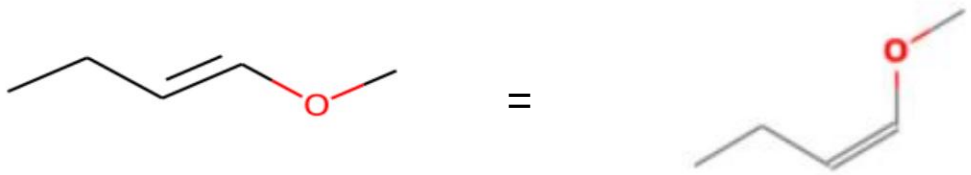

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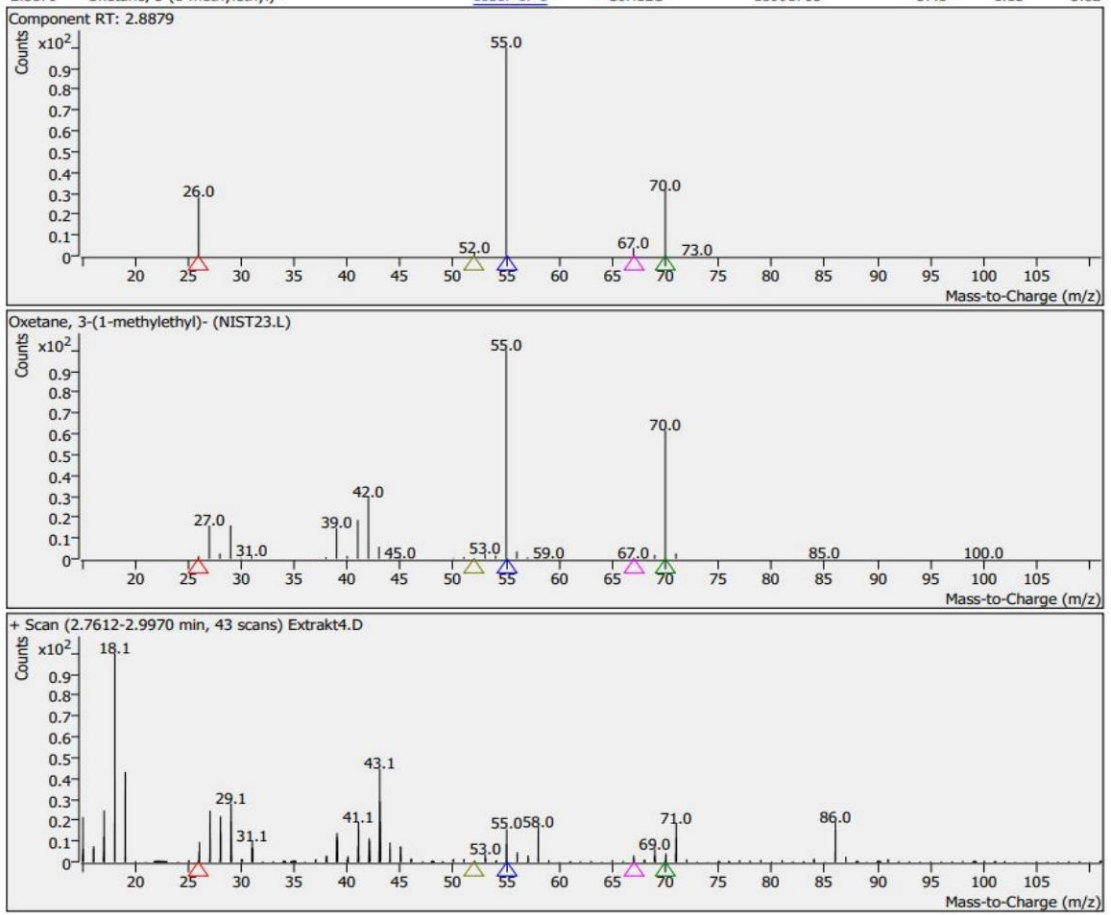
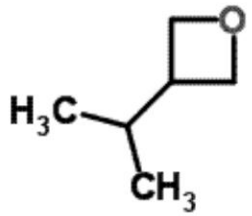
Oxetan, 3-(1-methyletyl)-, CAS 10317-17-6 / Peak RT: 2,8879 [ÿ 1,15 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
2.8879	Oxetane, 3-(1-methylethyl)-	10317-17-6	C6H12O	18991705		57.1	1.15	3.82





1. Identification

1.1 GHS Product identifier

Product name 3-propan-2-yloxetane

1.2 Other means of identification

Product number -
Other names Oxetane,3-(1-methylethyl)

1.3 Recommended use of the chemical and restrictions on use

Identified uses For industry use only.
Uses advised against no data available

1.4 Supplier's details

Company XiXisys.com
Address XiXisys.com
Telephone XiXisys.com
Fax XiXisys.com

1.5 Emergency phone number

Emergency phone number -
Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

2. Hazard identification

2.1 Classification of the substance or mixture

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s) no data available
Signal word no data available
Hazard statement(s) no data available
Precautionary statement(s)
Prevention no data available
Response no data available
Storage no data available
Disposal no data available

2.3 Other hazards which do not result in classification

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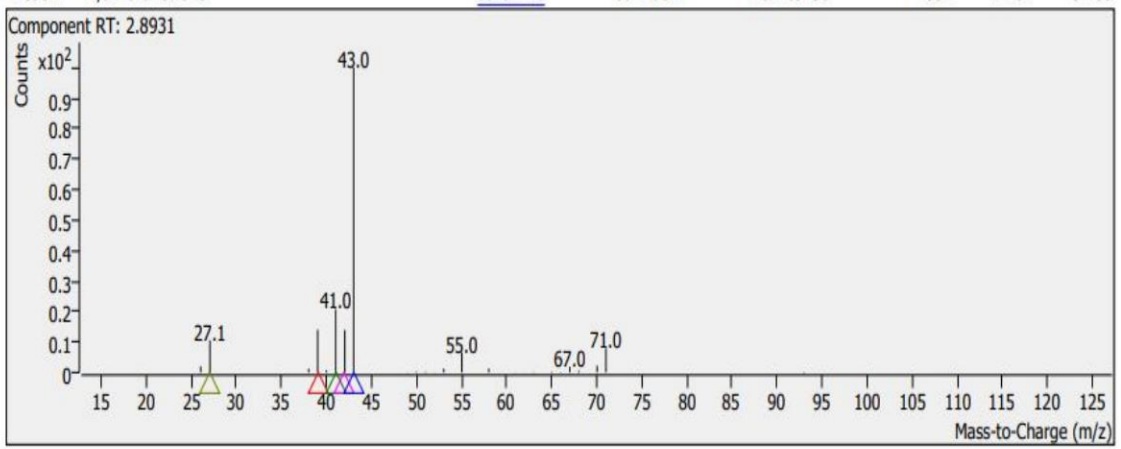
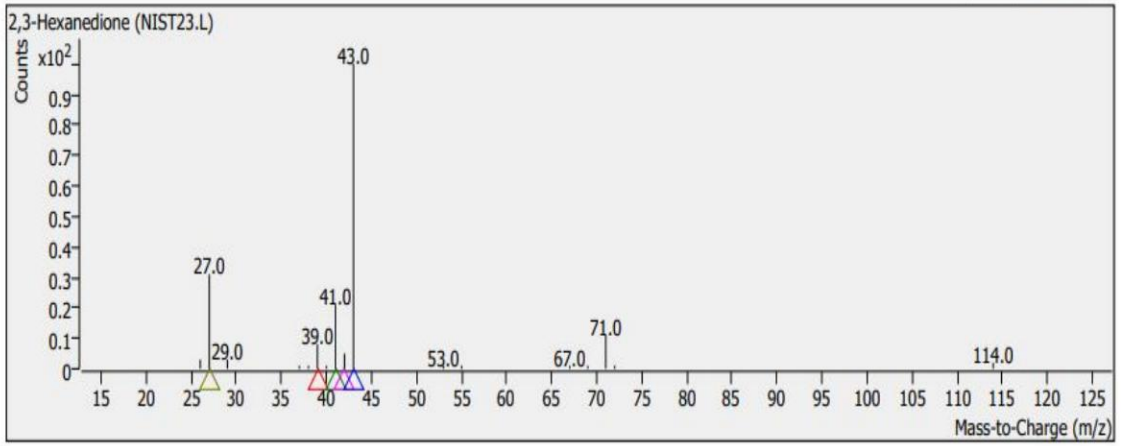
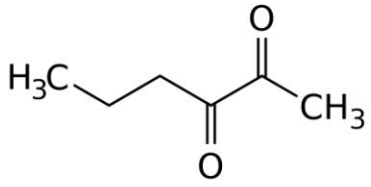
2,3-Hexadion, CAS 3848-24-6 / RT: 2,8931 [ÿ 28,0 areal%]

RT	Compound Name	CAS#	Formula	Area MI	Match Score	Sample	Sample
2.8931	2,3-Hexanedione	3848-24-6	C6H10O2	461289190	83.7	27.97	92.80







1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 2,3-Hexanedione

Product Number : W255807
Brand : Aldrich

CAS-No. : 3848-24-6

.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 3), H226

For the full text of the H-Statements mentioned in this Section, see Section 16.

.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Warning

Hazard statement(s)
H226 Flammable liquid and vapour.

Precautionary statement(s)

P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.

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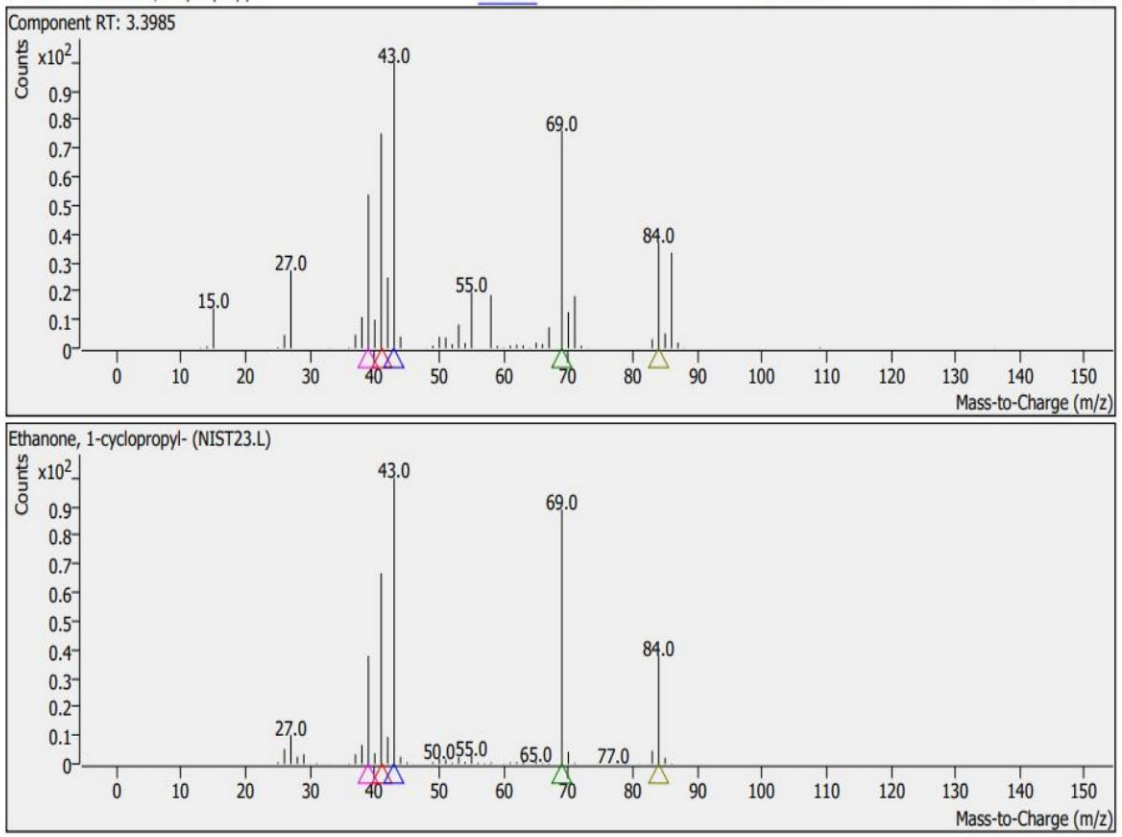
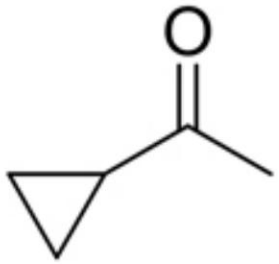
Ethanon, 1-cyclopropyl, CAS 765-43-5 / RT: 3,3985 [ÿ 30,1 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
3.3985	Ethanone, 1-cyclopropyl-	765-43-5	C5H8O	497053902		84.9	30.14	100.00





Cyclopropyl methyl ketone **Revision Date** 24-Dec-2021

Precautionary Statements
Prevention
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Skin
If skin irritation occurs: Get medical advice/attention
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower
Wash contaminated clothing before reuse
Eyes
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention
Ingestion
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
Rinse mouth
Fire
In case of fire: Use CO2, dry chemical, or foam for extinction
Storage
Store locked up
Store in a well-ventilated place. Keep cool
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)
None identified

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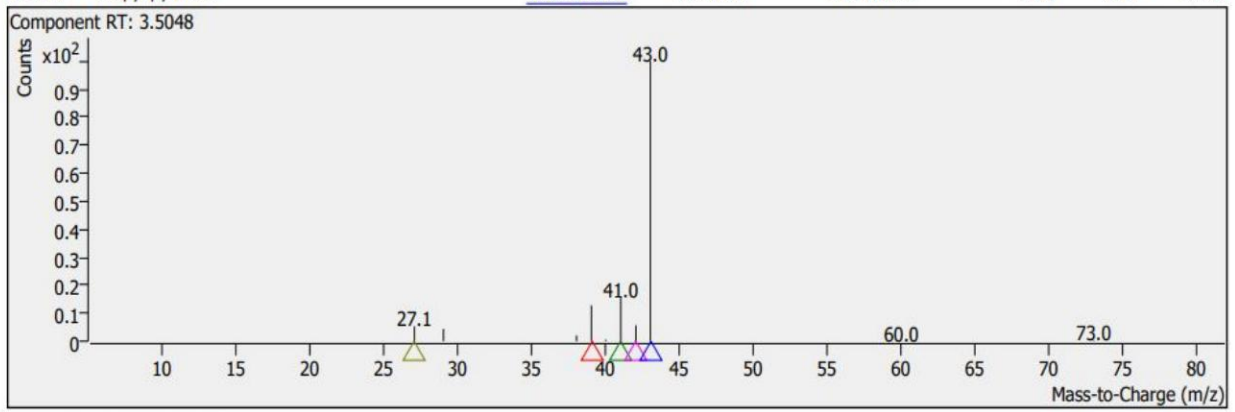
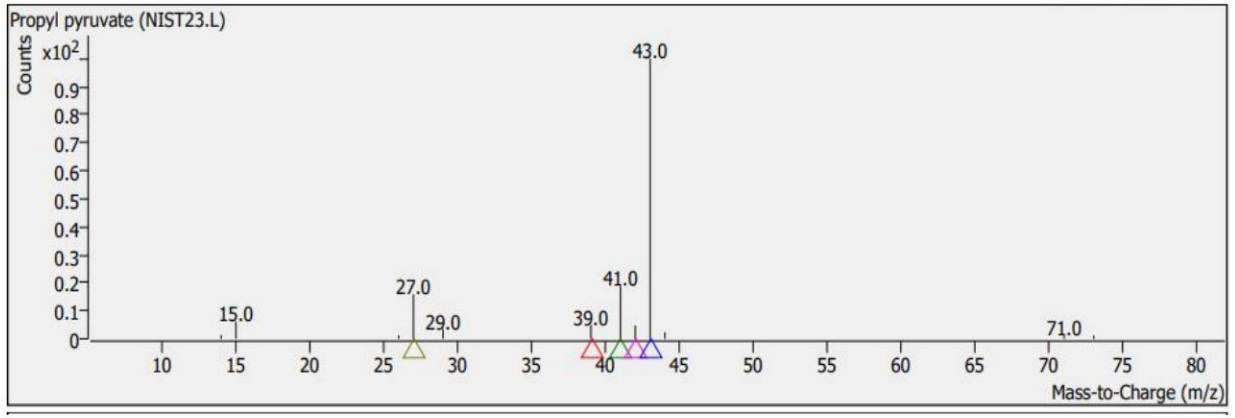
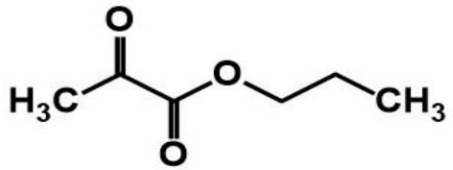
Propylpyruvat, CAS 1000431-41-8 / RT: 3,5048 [ÿ 7,8 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
3.5048	Propyl pyruvate	1000431-41-8	C6H10O3	129180976		87.8	7.83	25.99







Intet sikkerhedsdatablad fundet/til stede

Produktet er ikke klassificeret med hensyn til faresætning

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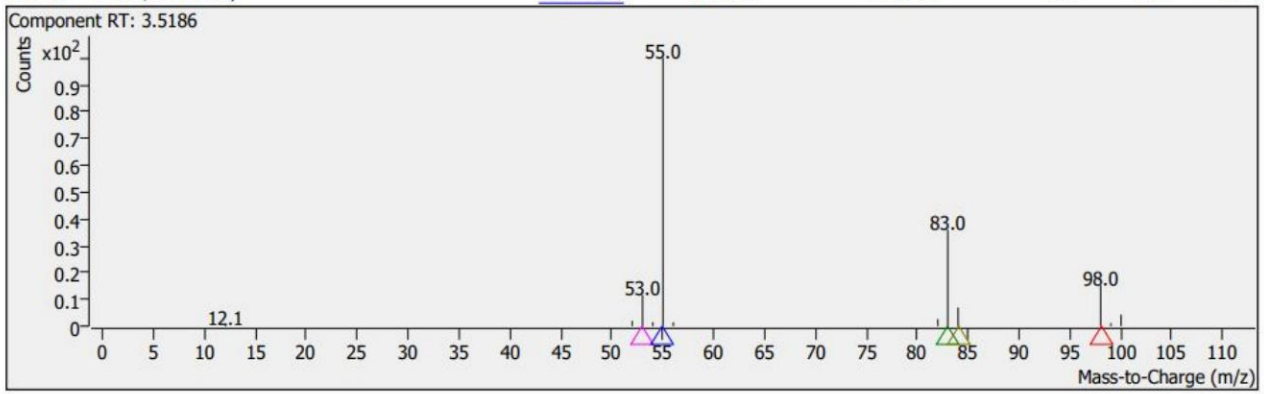
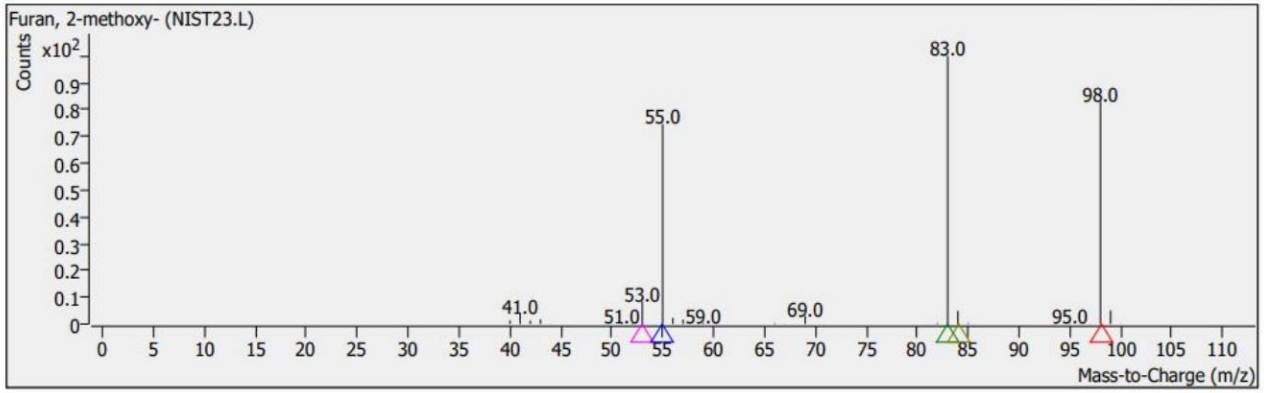
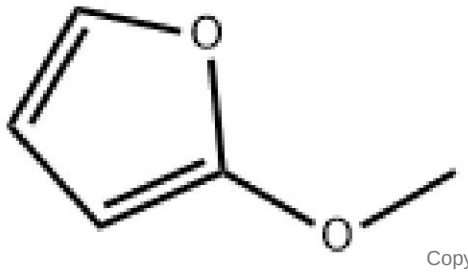
Machine Translated by Google

Furan, 2-methoxy-, CAS 25414-22-6 / RT: 3,5186 [ÿ 0,5 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
3.5186	Furan, 2-methoxy-	25414-22-6	C5H6O2	8759503		82.7	0.53	1.76







2-Methoxyfuran **Revision Date** 29-Mar-2024

Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Wear protective gloves/protective clothing/eye protection/face protection
Avoid breathing dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Keep cool

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Call a POISON CENTER or doctor/physician

Skin

Call a POISON CENTER or doctor/physician if you feel unwell
Wash contaminated clothing before reuse
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

Ingestion

IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
Rinse mouth

Fire

In case of fire: Use CO2, dry chemical, or foam for extinction

Storage

Store locked up
Store in a well-ventilated place. Keep container tightly closed

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

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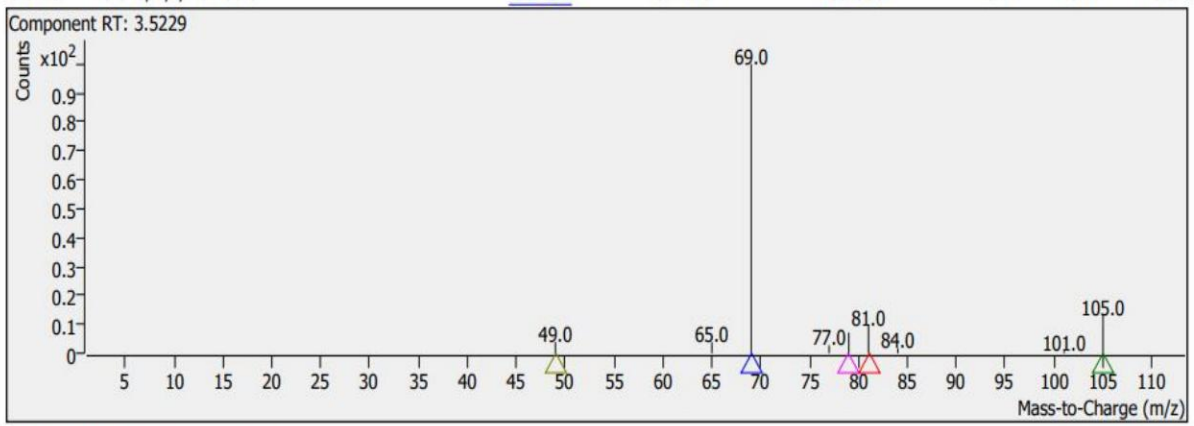
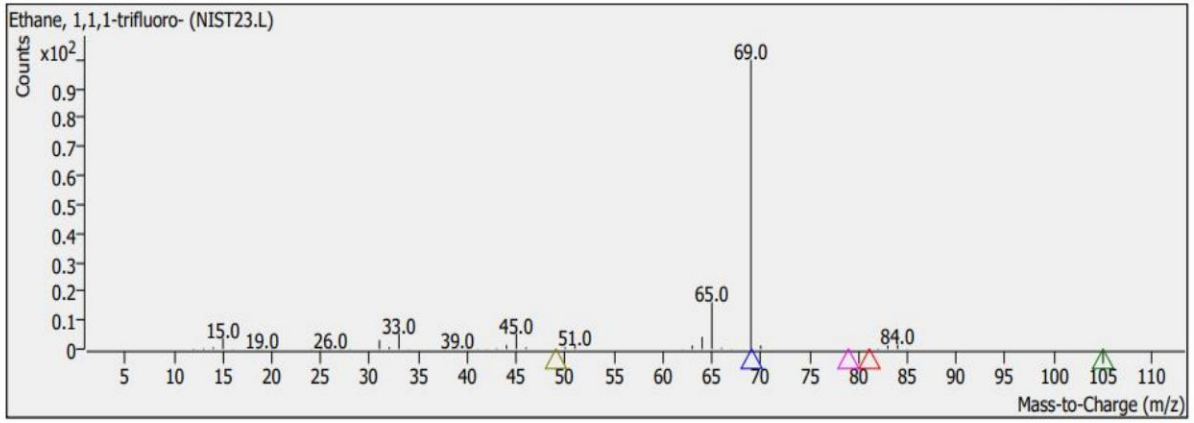
Ethan, 1,1,1-trifluor-, CAS 420-46-2 / RT: 3,5229 [ÿ 0,1 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
3.5229	Ethane, 1,1,1-trifluoro-	420-46-2	C2H3F3	1837998		52.1	0.11	0.37





Section 2. Hazards identification

OSHA/HCS status : This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Classification of the substance or mixture : GASES UNDER PRESSURE - Liquefied gas

GHS label elements

Hazard pictograms :

Signal word : Warning

Hazard statements : Contains gas under pressure; may explode if heated.
May cause frostbite.
May displace oxygen and cause rapid suffocation.

Precautionary statements

General : Read and follow all Safety Data Sheets (SDS'S) before use. Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand. Close valve after each use and when empty. Use equipment rated for cylinder pressure. Do not open valve until connected to equipment prepared for use. Use a back flow preventative device in the piping. Use only equipment of compatible materials of construction. Always keep container in upright position.

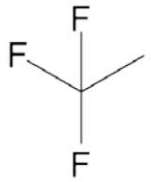
Prevention : Not applicable.

Response : Not applicable.

Storage : Protect from sunlight. Store in a well-ventilated place.

Disposal : Not applicable.

Hazards not otherwise classified : Liquid can cause burns similar to frostbite.



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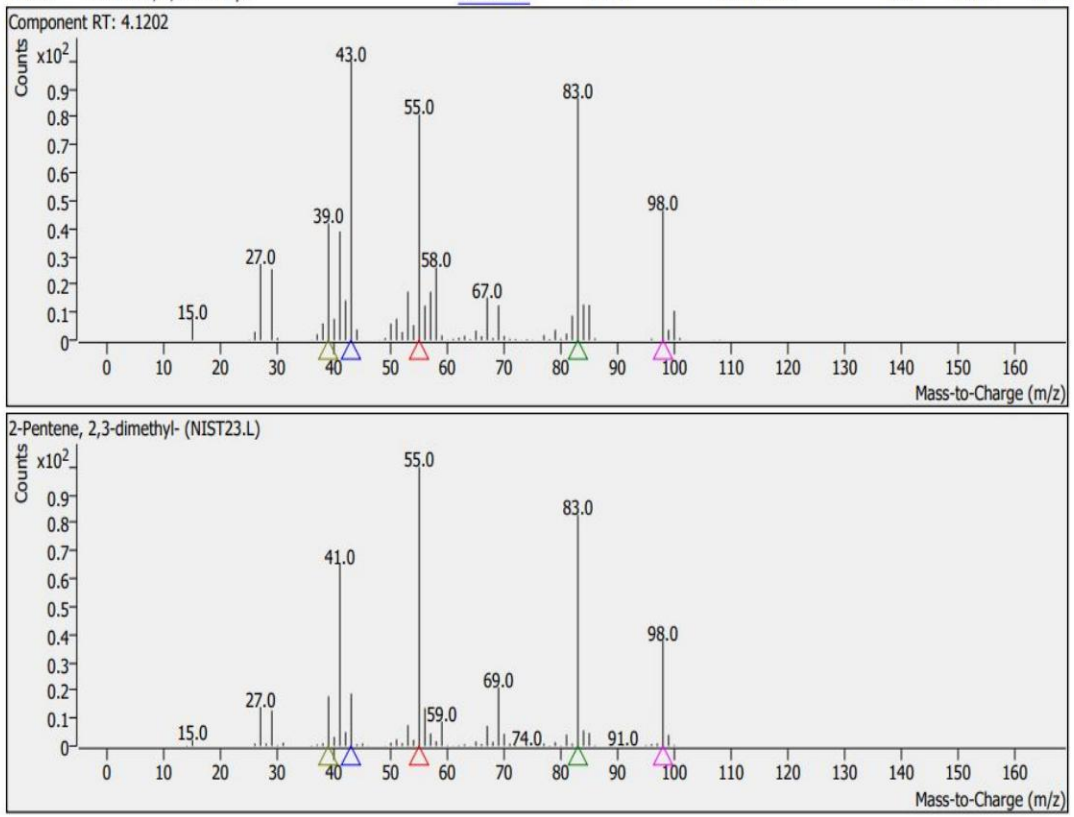
Machine Translated by Google

2-Penten, 2,3-dimethyl-, CAS 10574-37-5 / RT: 4,12 [ÿ 12,1 areal%]

RT	Compound Name	CAS#	Formula	Area MI	Match Score	Sample	Sample
4.1202	2-Pentene, 2,3-dimethyl-	10574-37-5	C7H14	199000520	89.9	12.07	40.04



2. Hazard identification

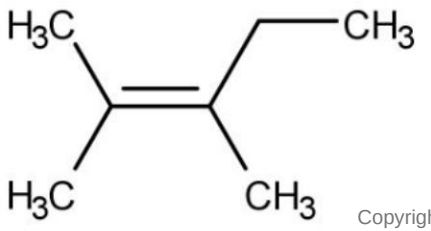
2.1 Classification of the substance or mixture

Flammable liquids, Category 2
Aspiration hazard, Category 1

2.2 GHS label elements, including precautionary statements

Pictogram(s)

Signal word	Danger
Hazard statement(s)	H225 Highly flammable liquid and vapour
	H304 May be fatal if swallowed and enters airways
Precautionary statement(s)	
Prevention	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
	P233 Keep container tightly closed.
	P240 Ground and bond container and receiving equipment.
	P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
	P242 Use non-sparking tools.
	P243 Take action to prevent static discharges.
	P280 Wear protective gloves/protective clothing/eye protection/face protection.
Response	P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].
	P370+P378 In case of fire: Use ... to extinguish.
	P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor/…
	P331 Do NOT induce vomiting.



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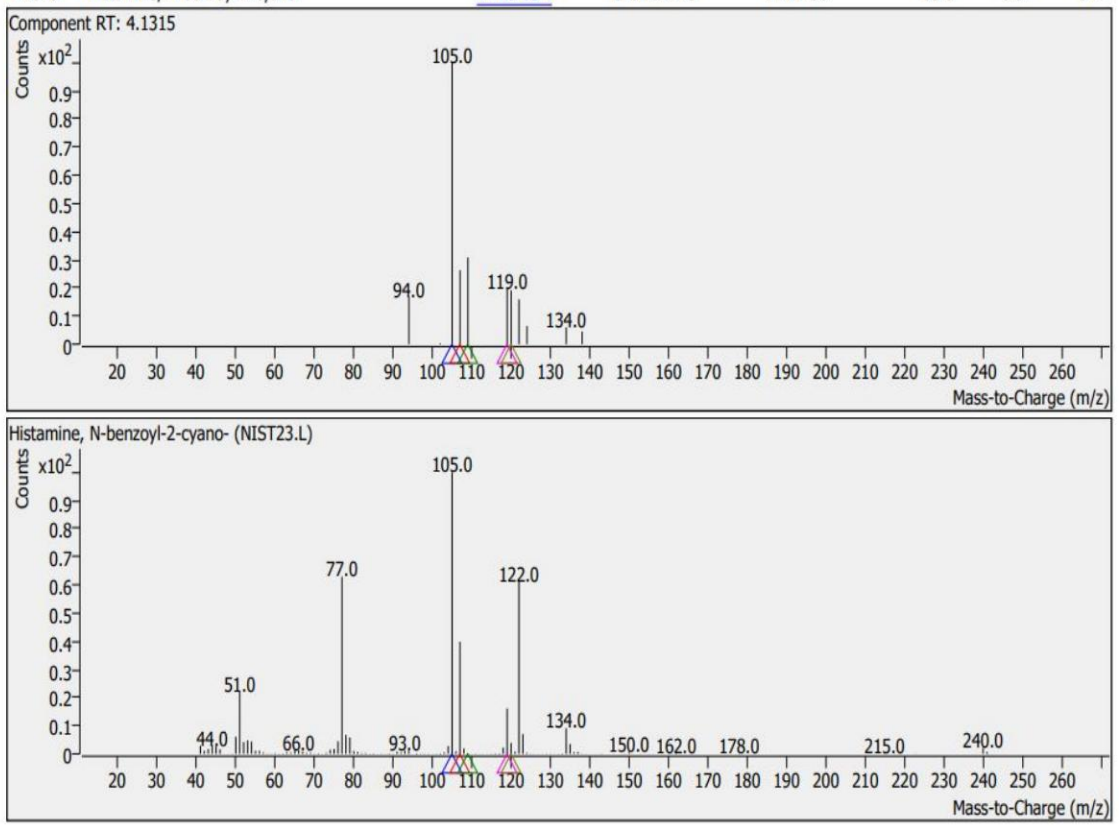
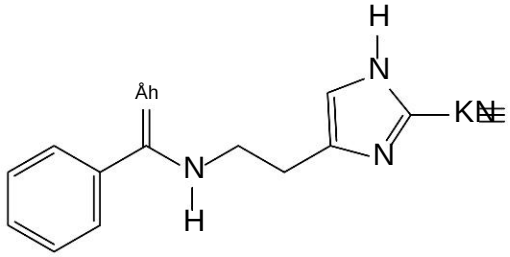
Machine Translated by Google

Histamin, N-benzoyl-2-cyano, CAS 74419-68-4/ RT: 4,1315 [ÿ 0,1 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
4.1315	Histamine, N-benzoyl-2-cyano-	74419-68-4	C13H12N4O	1211450		53.5	0.07	0.24





Histamine

Article Talk

From Wikipedia, the free encyclopedia

For the use as an immunostimulant drug, see Histamine dihydrochloride.

Histamine is an organic nitrogenous compound involved in local immune responses communication, as well as regulating physiological functions in the gut and acting as a neurotransmitter for the brain, spinal cord, and uterus.[3][4] Discovered in 1910, histamine has been considered a local hormone (autocoid) because it's produced without involvement of the classic endocrine glands; however, in recent years, histamine has been recognized as a central neurotransmitter.[5] Histamine is involved in the inflammatory response and has a central role as a mediator of itching.[6] As part of an immune response to foreign pathogens, histamine is produced by basophils and by mast cells found in nearby connective tissues. Histamine increases the permeability of the capillaries to white blood cells and some proteins, to allow them to engage pathogens in the infected tissues.[7] It consists of an imidazole ring attached to an ethylamine chain; under physiological conditions, the amino group of the side-chain is protonated.

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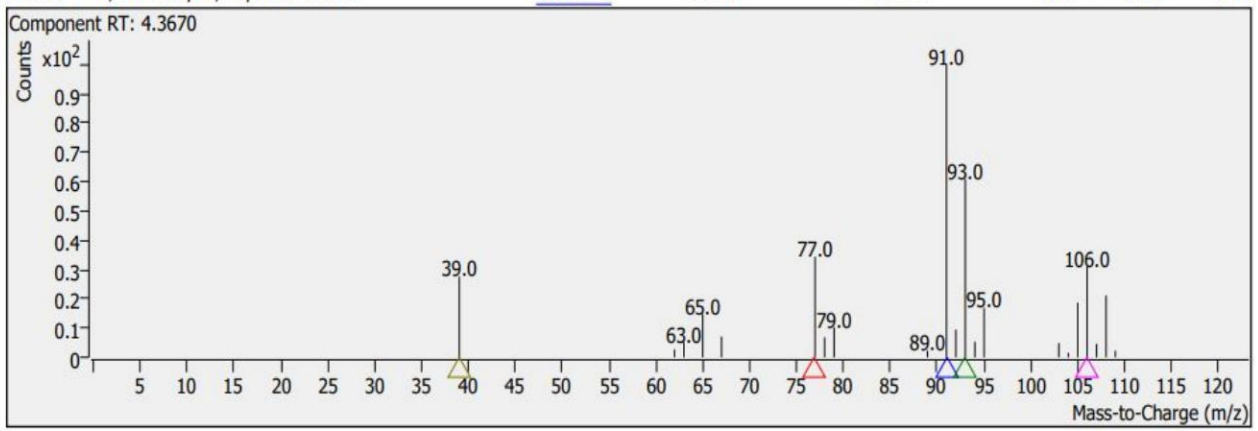
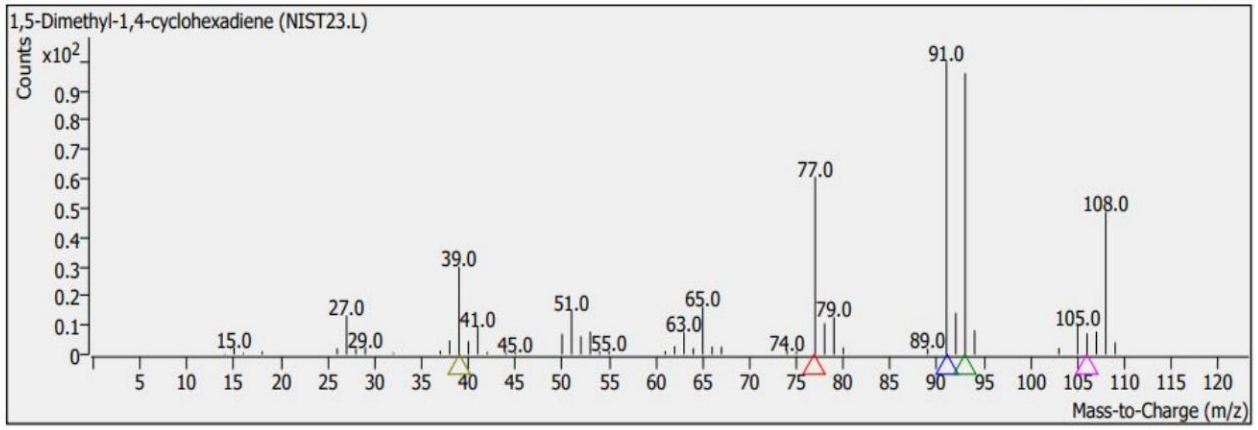
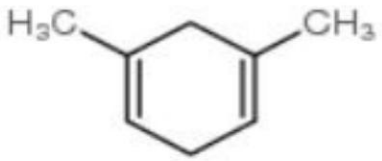
Machine Translated by Google

1,5-Dimethyl-1,4-cyclohexadien, CAS 4190-06-1 / RT: 4,3670 [ÿ 0,3 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
4.3670	1,5-Dimethyl-1,4-cyclohexadiene	4190-06-1	C8H12	4562178		82.0	0.28	0.92







1,5-DIMETHYL-1,4-CYCLOHEXADIENE SDS

SAFETY DATA SHEETS

According to Globally Harmonized System of Classification and Labelling of Chemicals (GHS) - Sixth revised edition

Version: 1.0

Creation Date: Aug 14, 2017

Revision Date: Aug 14, 2017

1.Identification

1.1 GHS Product identifier

Product name	1,5-dimethylcyclohexa-1,4-diene

1.2 Other means of identification

Product number	-
Other names	1,5-dimethyl-cyclohexa-1,4-diene

1.3 Recommended use of the chemical and restrictions on use

Identified uses	For industry use only.
Uses advised against	no data available

Yderligere detaljer fra SS, LookChem

Adobe Acrobat Document

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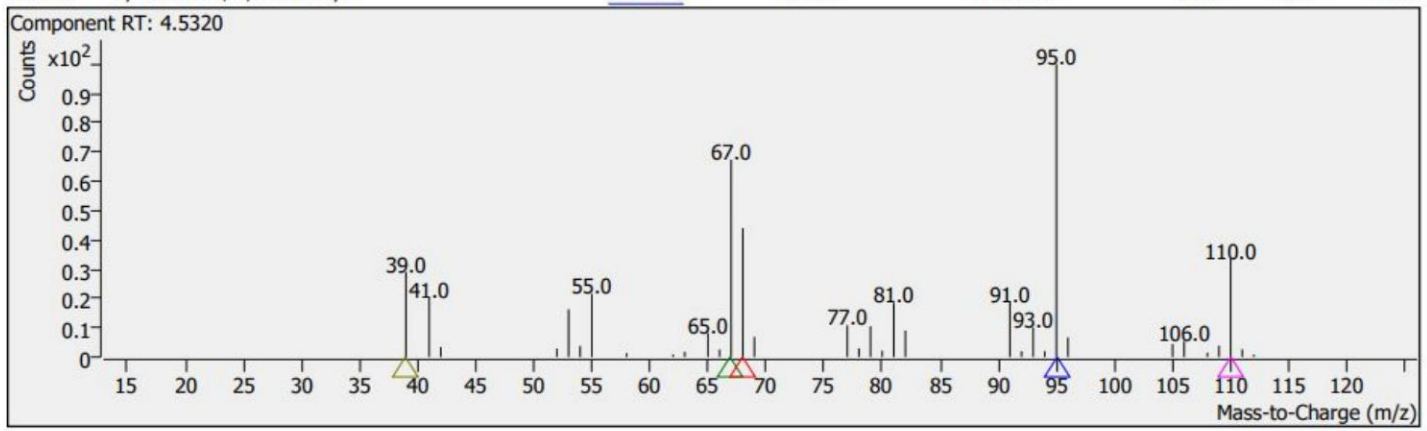
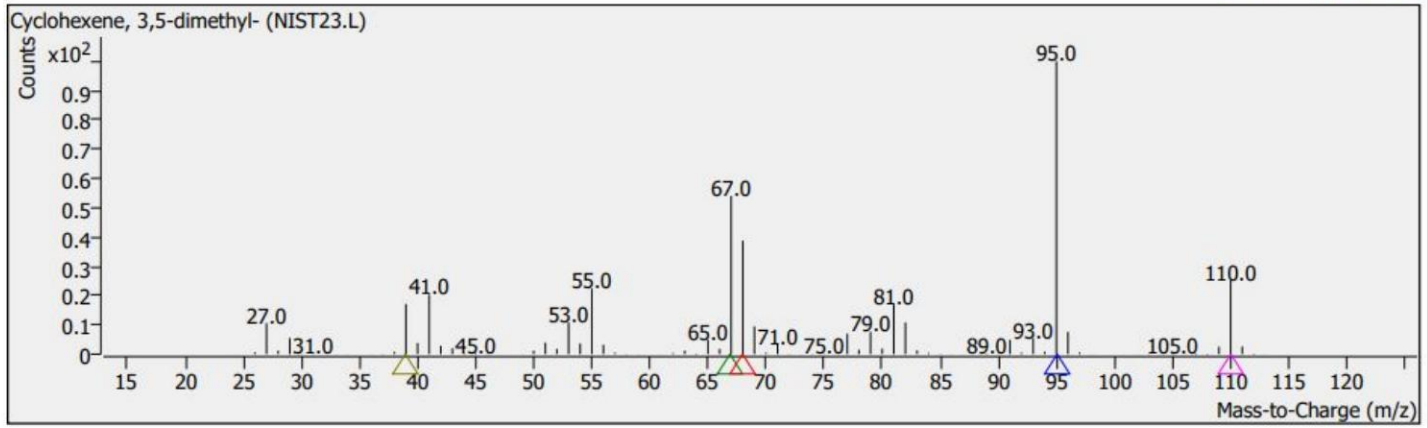
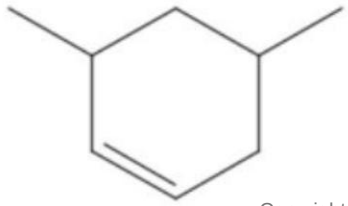
Machine Translated by Google

Cyclohexen, 3,5-dimethyl-, CAS 823-17-6 / RT: 4,5420 [ÿ 0,8 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
4.5320	Cyclohexene, 3,5-dimethyl-	823-17-6	C8H14	12650158		90.8	0.77	2.55







3,5-dimethylcyclohexene SDS

SAFETY DATA SHEETS

According to Globally Harmonized System of Classification and Labelling of Chemicals (GHS) - Sixth revised edition

Version: 1.0

Creation Date: Aug 18, 2017

Revision Date: Aug 18, 2017

1.Identification

1.1 GHS Product identifier

Product name	3,5-dimethyl-cyclohexene

1.2 Other means of identification

Product number	-
Other names	3,5-Dimethylcyclohexene

1.3 Recommended use of the chemical and restrictions on use

Identified uses	For industry use only.
Uses advised against	no data available

Yderligere detaljer fra SDS, LookChem

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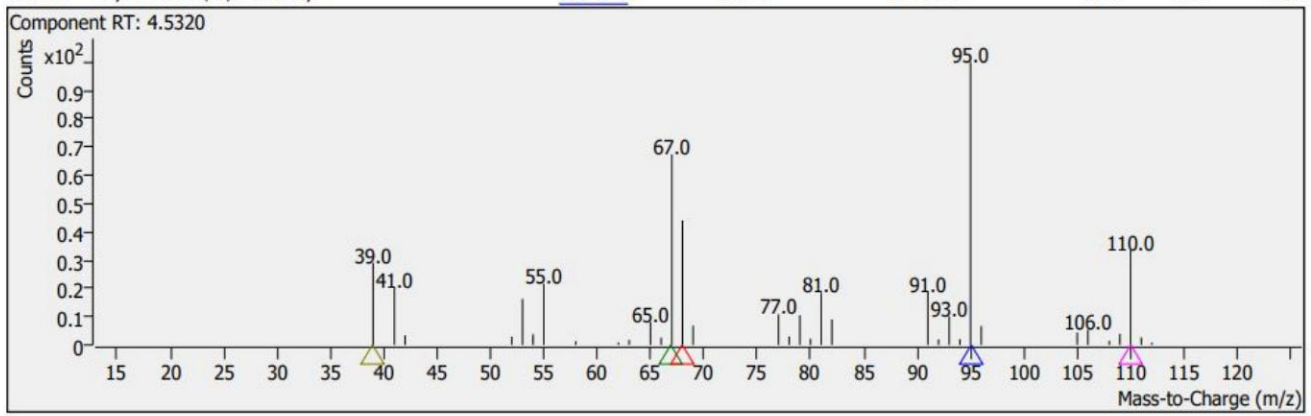
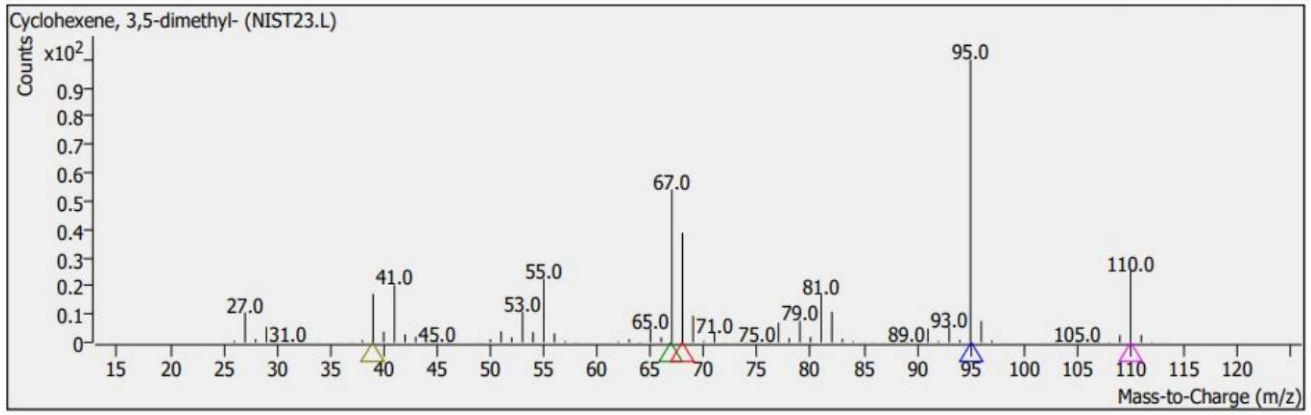
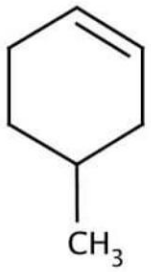
Machine Translated by Google

Cyclohexen, 4-methyl-, CAS 591-47-9 / RT: 4,5359 [ÿ 0,4 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
4.5320	Cyclohexene, 3,5-dimethyl-	823-17-6	C8H14	12650158		90.8	0.77	2.55







SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 2)	H225: Highly flammable liquid and vapor.
Skin irritation, (Category 2)	H315: Causes skin irritation.
Eye irritation, (Category 2)	H319: Causes serious eye irritation.

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Specific target organ toxicity - single exposure, (Category 3), Respiratory system	H335: May cause respiratory irritation.
Aspiration hazard, (Category 1)	H304: May be fatal if swallowed and enters airways.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
Precautionary Statements	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P301 + P310 + P331	IF SWALLOWED: Immediately call a POISON CENTER/doctor. Do NOT induce vomiting.
P302 + P352	IF ON SKIN: Wash with plenty of water.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:
The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
Toxicological information:
The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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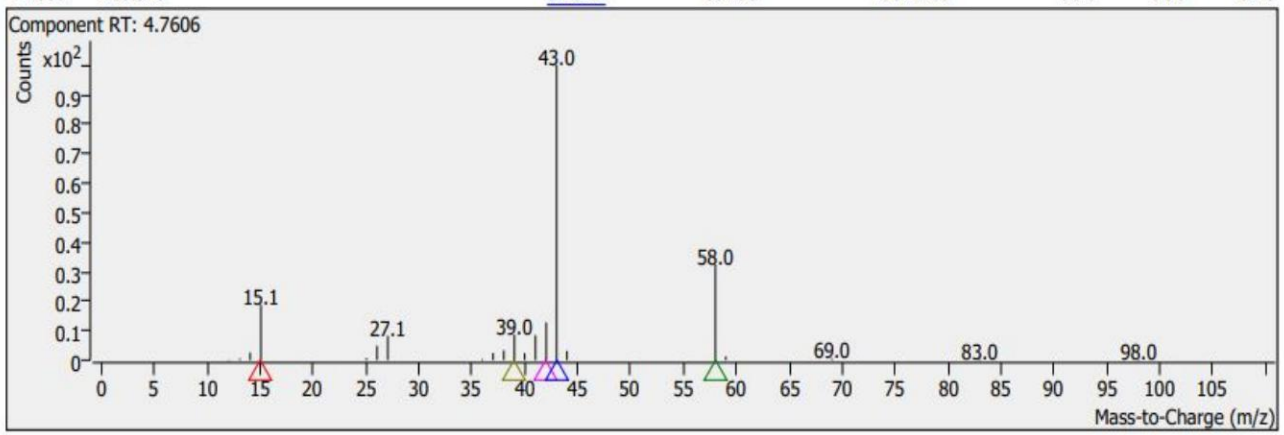
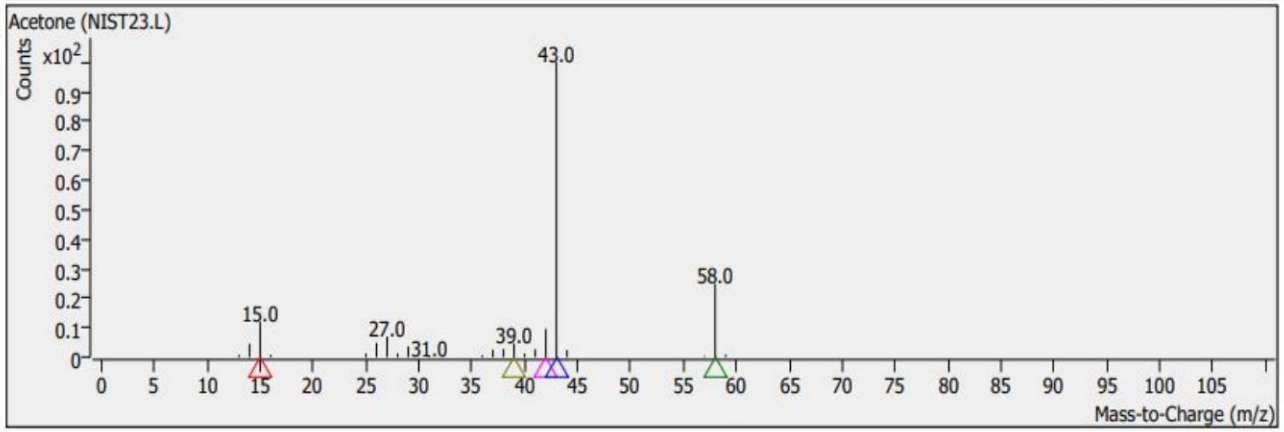
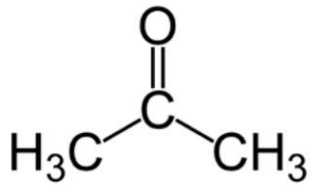
Aceton, CAS 67-64-1 / RT: 4,7606 [ÿ 1,0 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
4.7606	Acetone	67-64-1	C3H6O	15824489		95.0	0.96	3.18







SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 2)	H225: Highly flammable liquid and vapor.
Eye irritation, (Category 2)	H319: Causes serious eye irritation.
Specific target organ toxicity - single exposure, (Category 3), Central nervous system	H336: May cause drowsiness or dizziness.

The life science business of Merck operates as MilliporeSigma in the US and Canada

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
Hazard Statements	
H225	Highly flammable liquid and vapor.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
Precautionary Statements	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use non-sparking tools.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard information (EU)	
EUH066	Repeated exposure may cause skin dryness or cracking.

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:
The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
Toxicological information:
The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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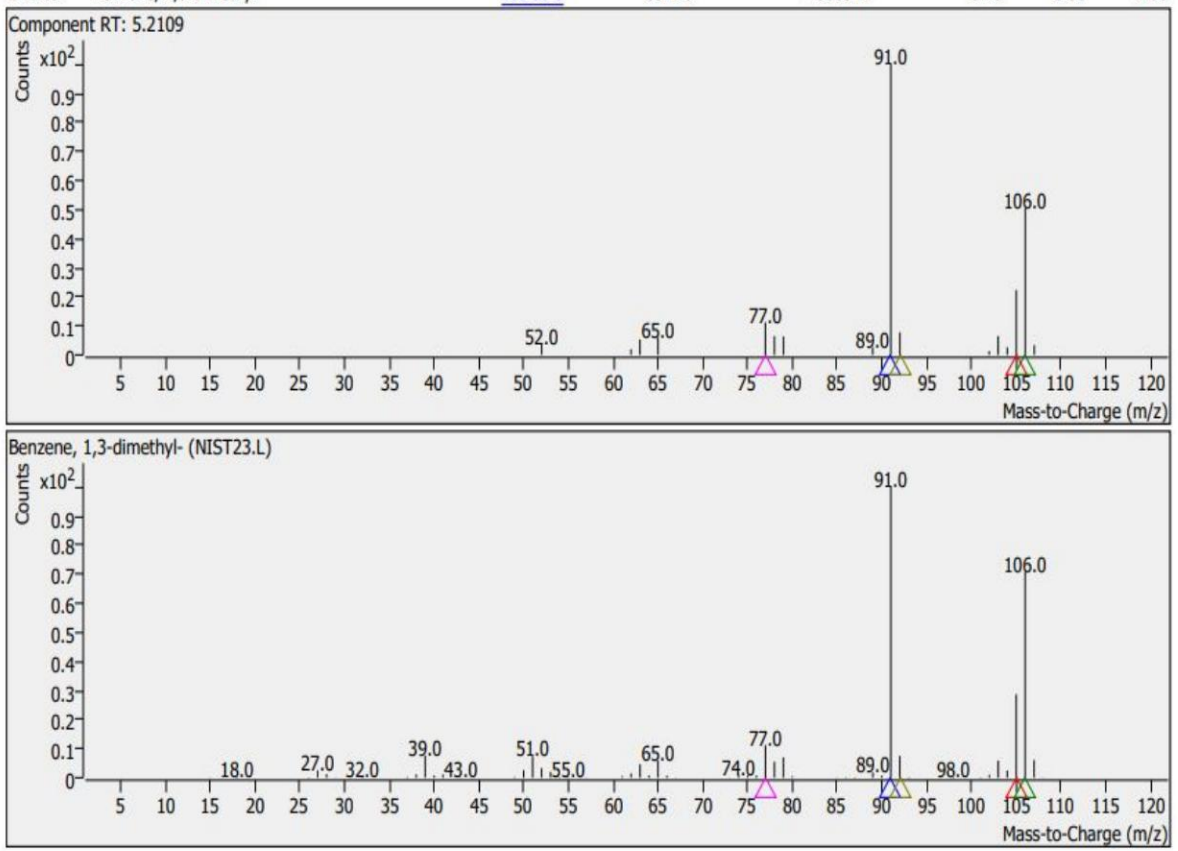
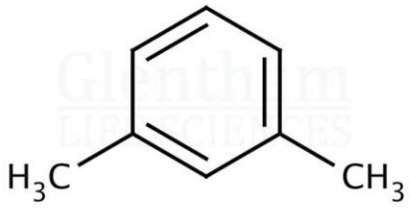
Benzen, 1,2-dimethyl-, CAS 108-38-3 / RT = 5,2109 [ÿ 0,3 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
5.2109	Benzene, 1,3-dimethyl-	108-38-3	C8H10	4990927		92.9	0.30	1.00





SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008
Flammable liquids (Category 3), H226
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315
Eye irritation (Category 2), H319
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Aspiration hazard (Category 1), H304
Chronic aquatic toxicity (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008
Pictogram

Signal word: Danger

Hazard statement(s)

H226	Flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H312 + H332	Harmful in contact with skin or if inhaled
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H412	Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P261	Avoid breathing vapours.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P331	Do NOT induce vomiting.
Supplemental Hazard Statements	none

2.3 Other hazards
This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	:	1,3-Dimethylbenzene
Formula	:	C_8H_{10}
Molecular weight	:	106.17 g/mol
CAS-No.	:	108-38-3
EC-No.	:	203-576-3
Index-No.	:	601-022-00-9

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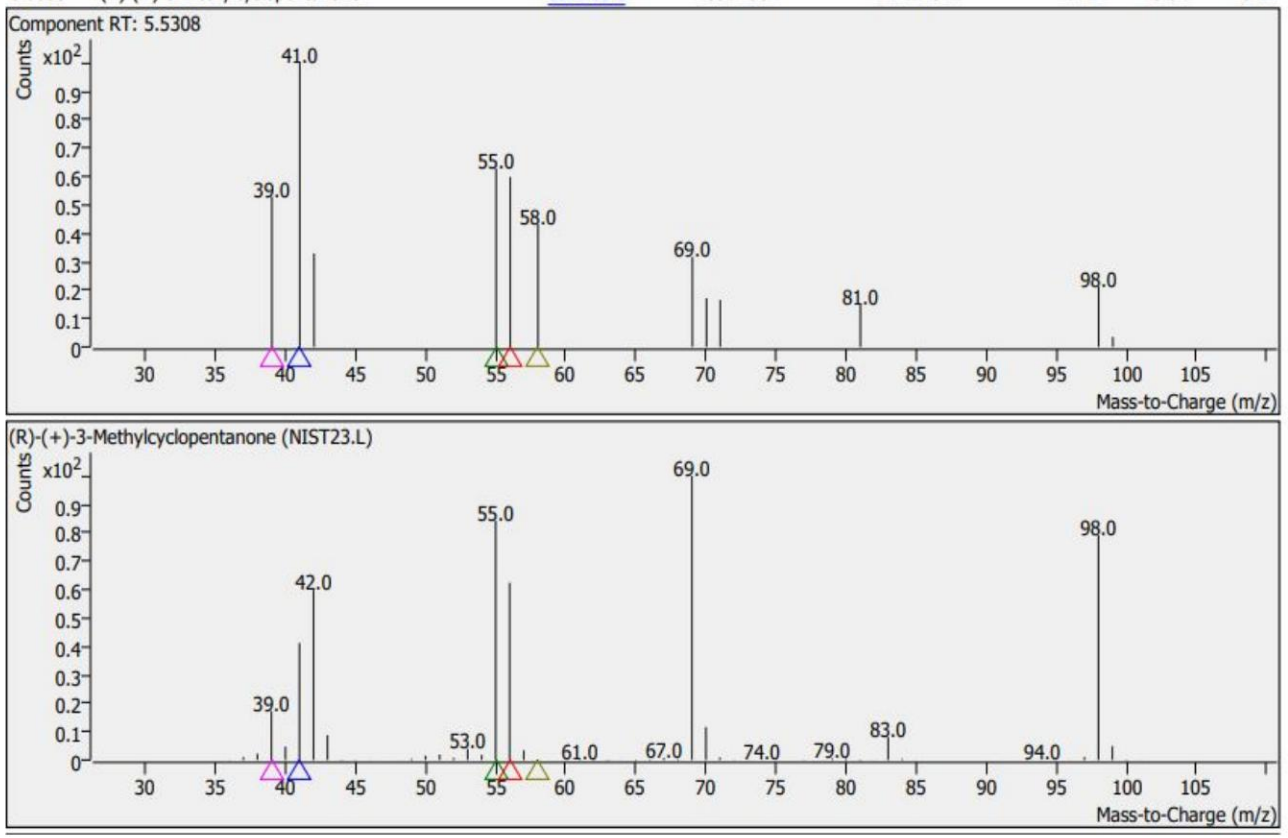
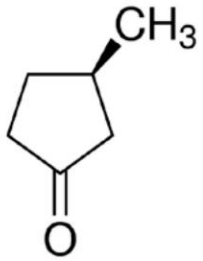
Machine Translated by Google

(R)-(+)-3-methylcyclopentanon, CAS 6672-30-6 / RT = 5,2484/5,5308 [ÿ 0,2 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
5.5308	(R)-(+)-3-Methylcyclopentanone	6672-30-6	C6H10O	1212191		74.2	0.07	0.24





Product identifier

Product name	: (R)-(+)-3-METHYLCYCLOPENTANONE
CBnumber	: CB9206841
CAS	: 6672-30-6
EINECS Number	: 229-711-6
Synonyms	: (R)-(+)-3-Methylcyclopentanone

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word: Warning

Hazard statements

H226 Flammable liquid and vapour

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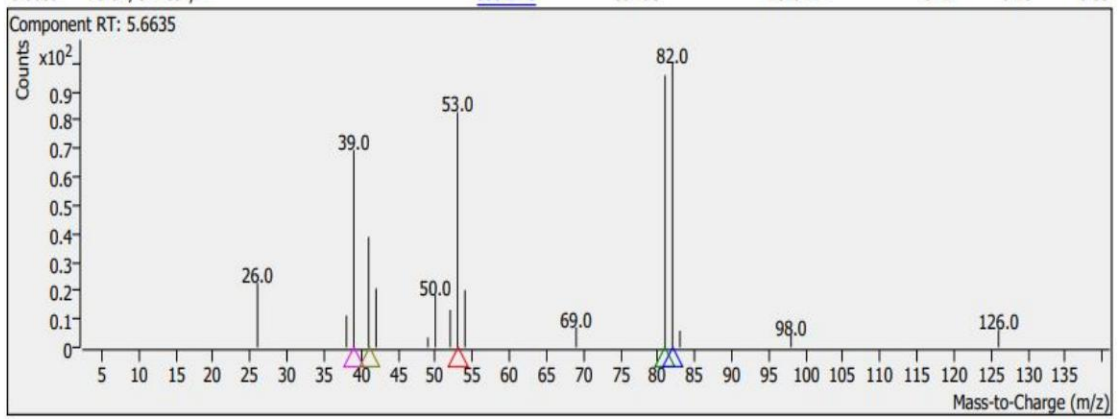
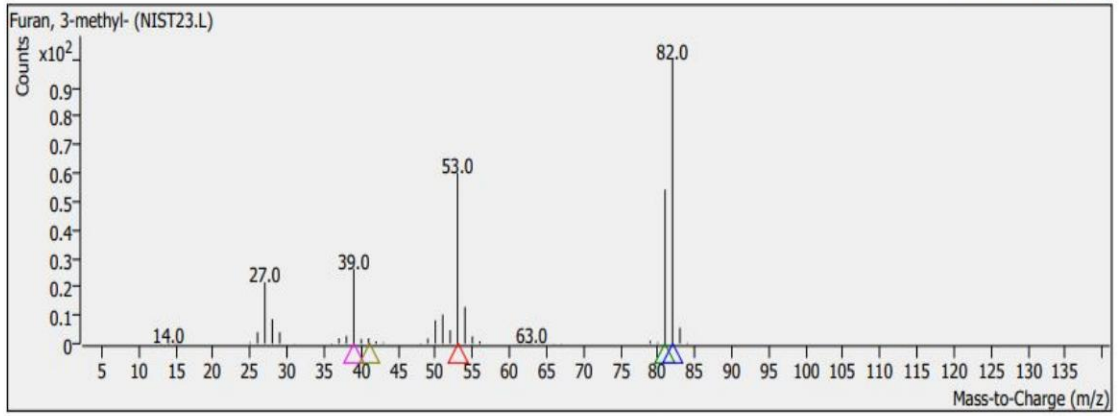
Machine Translated by Google

Furan, 3-methyl-, CAS 930-27-8 / RT = 5,6635 [ÿ 0,2 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
5.6635	Furan, 3-methyl-	930-27-8	C5H6O	2619124		81.2	0.16	0.53



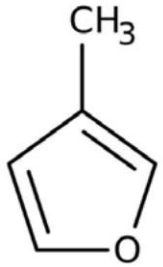


7.1 Hazards Identification

7.1.1 GHS Classification

Pictogram(s)	Acute Toxic Irritant
Signal	Danger
GHS Hazard Statements	H302 (92.68%): Harmful if swallowed [Warning Acute toxicity, oral] H331 (95.12%): Toxic if inhaled [Danger Acute toxicity, inhalation]
Precautionary Statement Codes	P261, P264, P270, P271, P301+P317, P304+P340, P316, P321, P330, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 44 reports by companies from 5 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 3 of 44 reports by companies. For more detailed information, please visit ECHA C&L website.* *Of the 4 notification(s) provided by 41 of 44 reports by companies with hazard statement code(s).* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)



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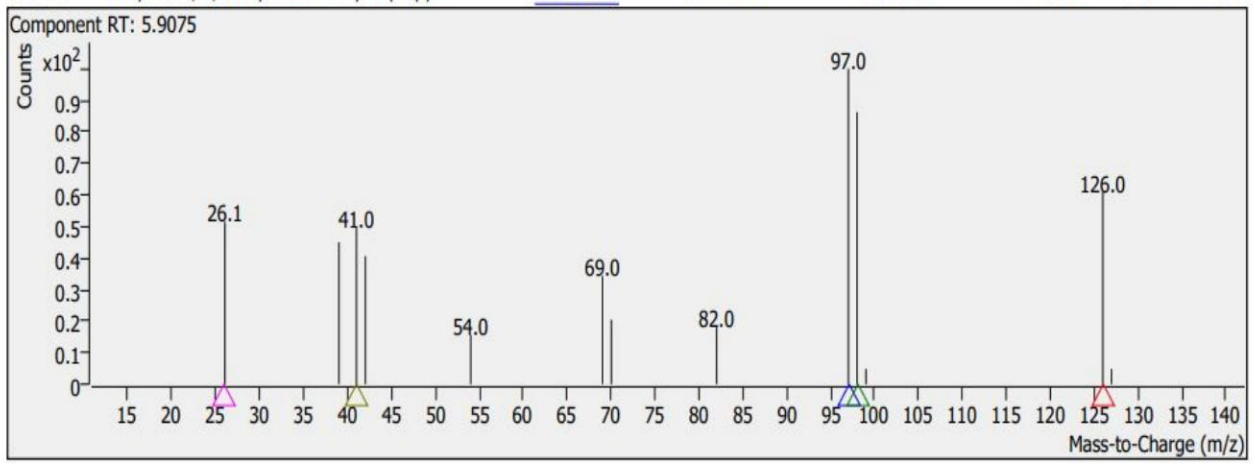
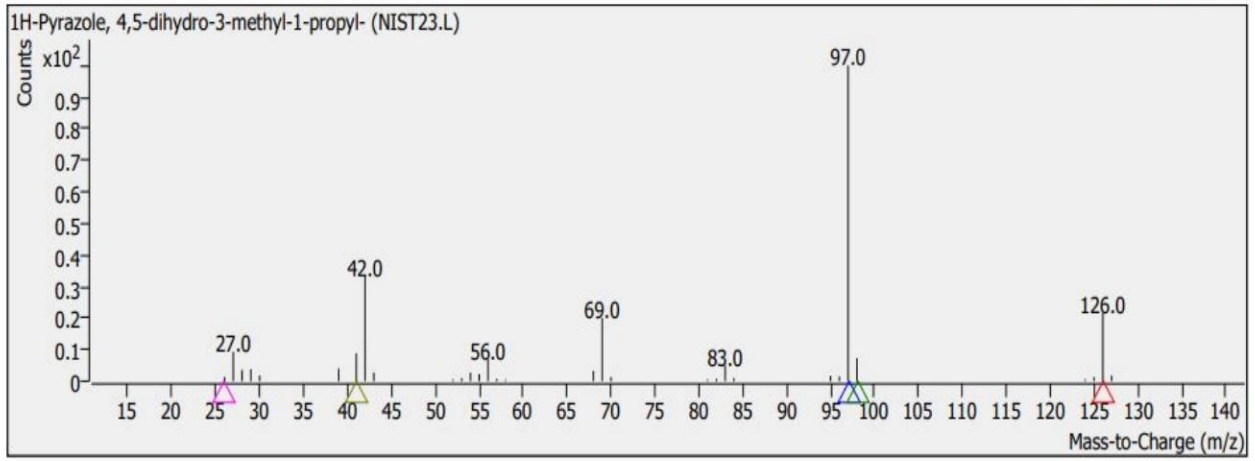
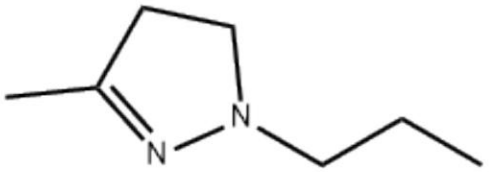
Machine Translated by Google

1H-Pyrazol, 4,5-dihydro-3methyl-1-propyl-, CAS 26964-49-8 / RT = 5,9075 [ÿ 0,1 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
5.9075	1H-Pyrazole, 4,5-dihydro-3-methyl-1-propyl-	26964-49-8	C7H14N2	1382050		75.0	0.08	0.28







2.Hazard identification

2.1 Classification of the substance or mixture

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s)	no data available
Signal word	no data available
Hazard statement(s)	no data available
Precautionary statement(s)	
Prevention	no data available
Response	no data available
Storage	no data available
Disposal	no data available

?

2.3 Other hazards which do not result in classification

no data available

3.Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
5-methyl-2-propyl-3,4-dihydropyrazole	5-methyl-2-propyl-3,4-dihydropyrazole	26964-49-8	none	100%

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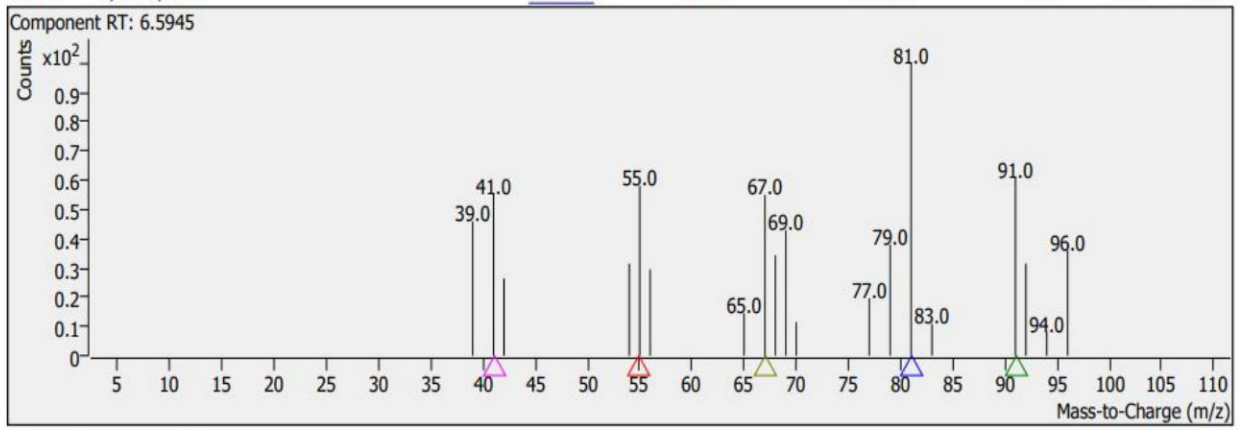
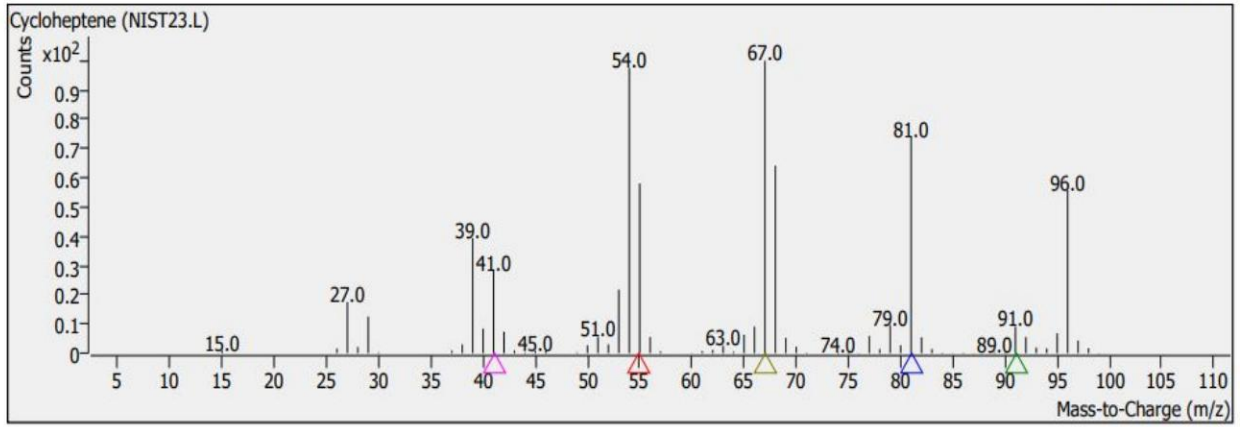
Machine Translated by Google

Cyclohepten, CAS 628-92-2 / RT = 6,5945 [ÿ 0,2 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
6.5945	Cycloheptene	628-92-2	C7H12	3017986		73.2	0.18	0.61





8 Safety and Hazards

8.1 Hazards Identification

8.1.1 GHS Classification

Pictogram(s)	Flammable
Signal	Danger
GHS Hazard Statements	H225 (100%): Highly Flammable liquid and vapor [Danger Flammable liquids]
Precautionary Statement Codes	P210, P233, P240, P241, P242, P243, P280, P303+P361+P353, P370+P378, P403+P235, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 75 reports by companies from 2 notifications to the ECHA C&L Inventory.* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

Synonyms	CYCLOHEPTENE 628-92-2 cis-Cycloheptene (Z)-Cycloheptene 45509-99-7 View More...
Molecular Weight	96.17 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-03-26 Modify: 2024-09-14
Description	Cycloheptene appears as a colorless oily liquid. Insoluble in water and less dense than water. Vapors heavier than air. Inhalation of high concentrations may have a narcotic effect. Used to make other chemicals.

▸ CAMEO Chemicals

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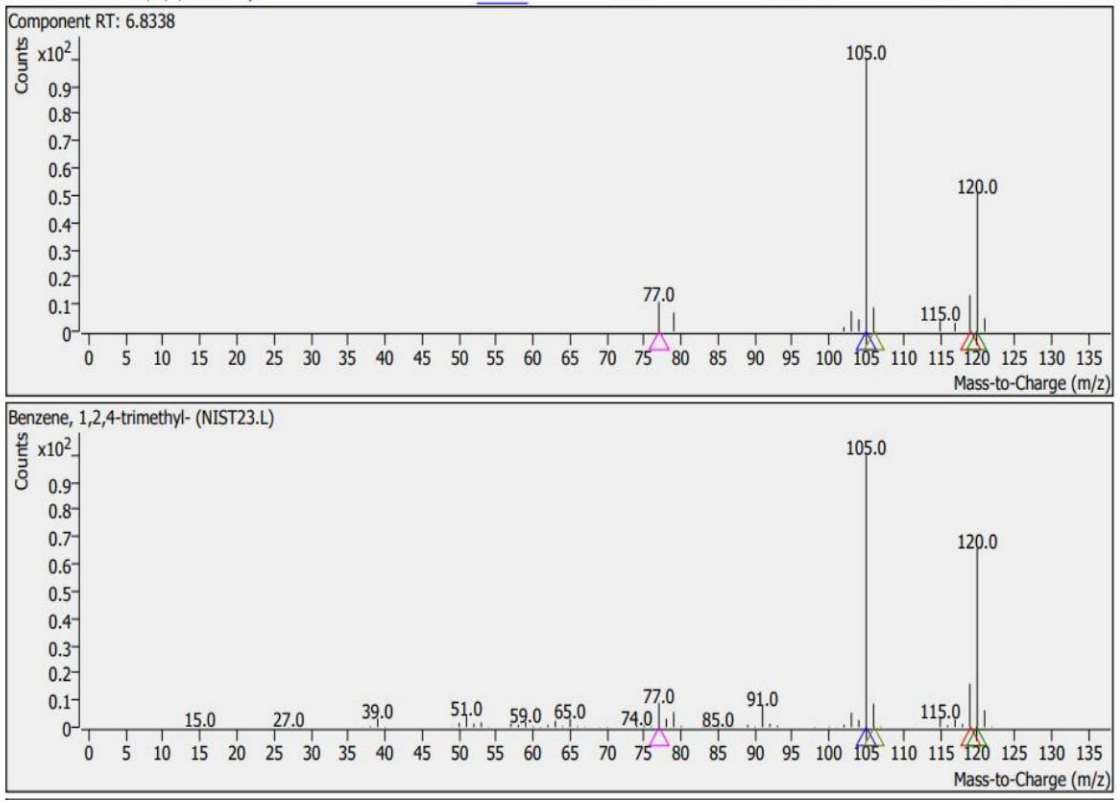
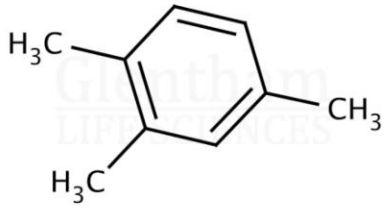
Benzen, 1,2,4-trimethyl-, CAS 95-63-6 / RT = 6,8338 [ÿ 0,1 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
6.8338	Benzene, 1,2,4-trimethyl-	95-63-6	C9H12	1466138		86.2	0.09	0.29





SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Flammable liquids (Category 3), H226
Acute toxicity, Inhalation (Category 4), H332
Skin irritation (Category 2), H315
Eye irritation (Category 2), H319
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Aspiration hazard (Category 1), H304
Long-term (chronic) aquatic hazard (Category 2), H411

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The life science business of Merck operates as MilliporeSigma in the US and Canada

1 GHS Classification

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Pictogram(s)	Flammable, Irritant, Health Hazard, Environmental Hazard
Signal	Danger
GHS Hazard Statements	H226 (100%): Flammable liquid and vapor [Warning Flammable liquids] H304 (10.5%): May be fatal if swallowed and enters airways [Danger Aspiration hazard] H315 (99.21%): Causes skin irritation [Warning Skin corrosion/irritation] H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H332 (99.97%): Harmful if inhaled [Warning Acute toxicity, inhalation] H335 (100%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation] H411 (99.31%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P210, P233, P240, P241, P242, P243, P261, P264, P264+P265, P271, P273, P280, P301+P316, P302+P352, P303+P361+P353, P304+P340, P305+P351+P338, P317, P319, P321, P331, P332+P317, P337+P317, P362+P364, P370+P378, P391, P403+P233, P403+P235, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 3183 companies from 57 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 2 of 3183 companies. For more detailed information, please visit ECHA C&L website.* *Of the 56 notification(s) provided by 3181 of 3183 companies with hazard statement code(s).* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

European Chemicals Agency (ECHA)

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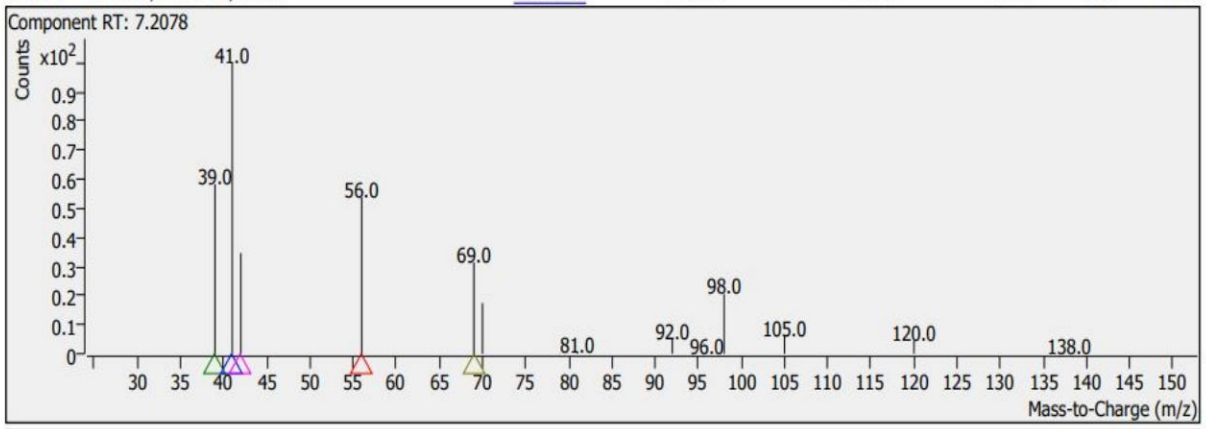
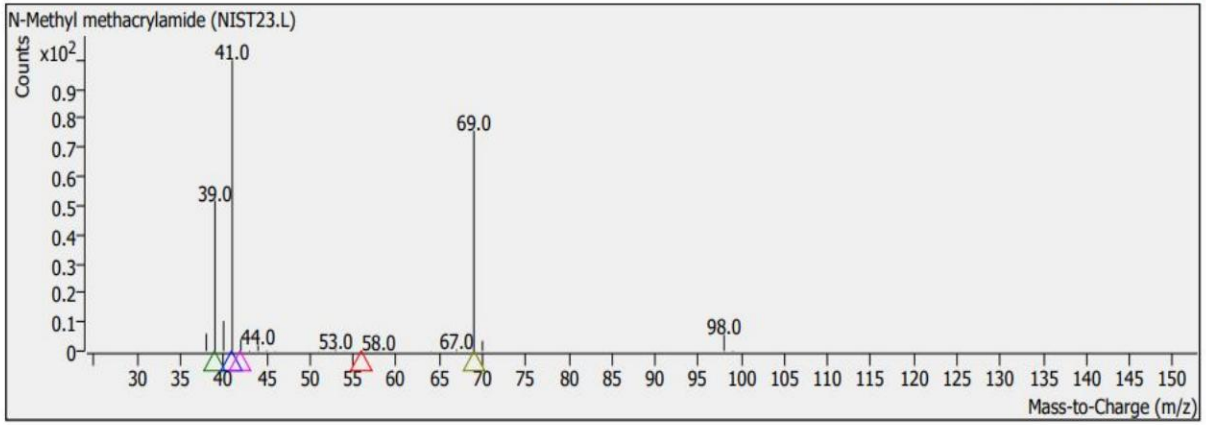
N-Methylmethacrylamid, CAS 3887-02-3 / RT = 7,2078 [ÿ 0,1 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
7.2078	N-Methyl methacrylamide	3887-02-3	C5H9NO	794861		68.5	0.05	0.16





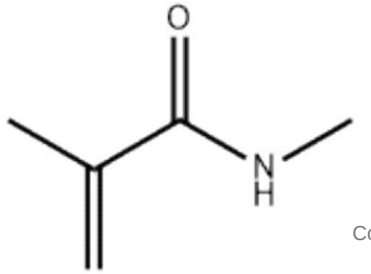
7 Safety and Hazards

7.1 Hazards Identification

7.1.1 GHS Classification

Pictogram(s)	Irritant
Signal	Warning
GHS Hazard Statements	H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation] H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H335 (100%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]
Precautionary Statement Codes	P261, P264, P264+P265, P271, P280, P302+P352, P304+P340, P305+P351+P338, P319, P321, P332+P317, P337+P317, P362+P364, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*The GHS information provided by 1 company from 1 notification to the ECHA C&L Inventory.*

▸ European Chemicals Agency (ECHA)



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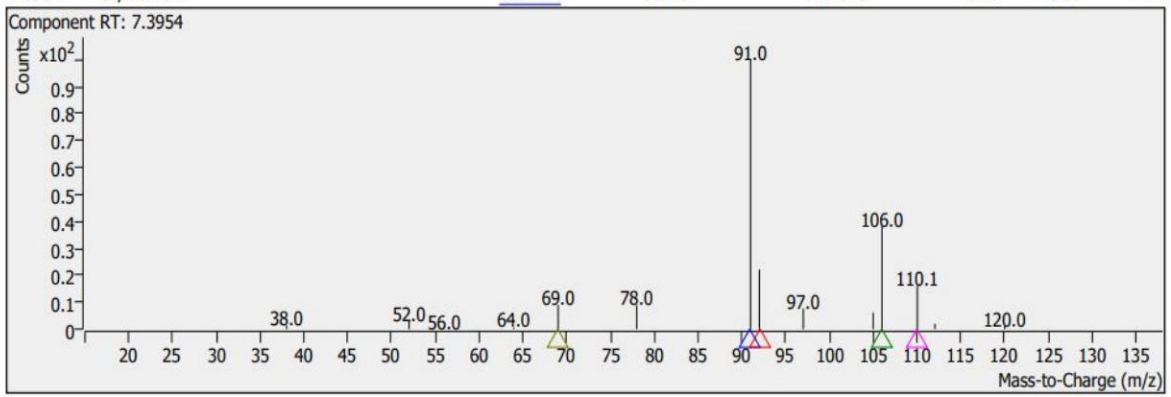
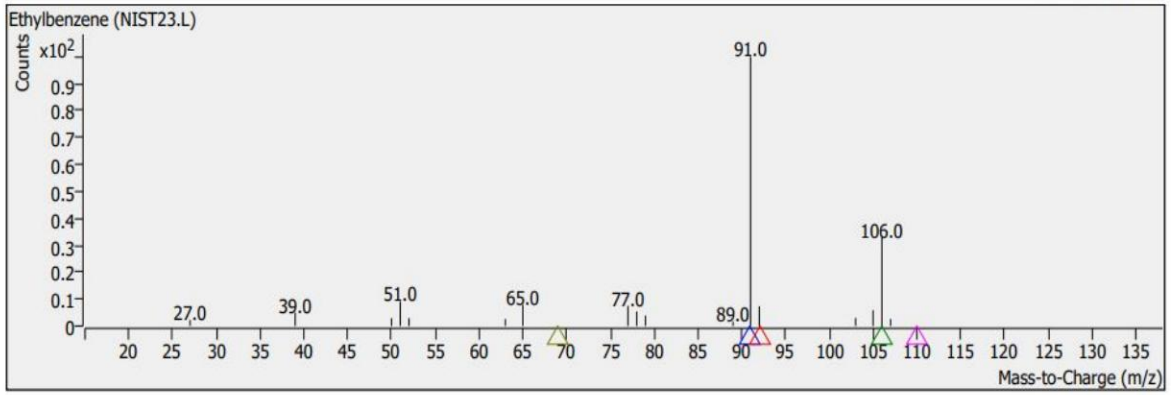
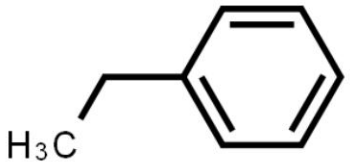
Ethylbenzen, CAS 100-41-4 / RT = 7,3954 [ÿ 0,4 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
7.3954	Ethylbenzene	100-41-4	C8H10	6184923		64.5	0.38	1.24







1 GHS Classification

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Pictogram(s)	Flammable, Irritant, Health Hazard
Signal	Danger
GHS Hazard Statements	H225 (99.97%): Highly Flammable liquid and vapor [Danger Flammable liquids] H304 (16.41%): May be fatal if swallowed and enters airways [Danger Aspiration hazard] H332 (99.91%): Harmful if inhaled [Warning Acute toxicity, inhalation] H373 (18.83%): May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure]
Precautionary Statement Codes	P210, P233, P240, P241, P242, P243, P260, P261, P271, P280, P301+P316, P303+P361+P353, P304+P340, P317, P319, P331, P370+P378, P403+P235, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 6991 companies from 68 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 2 of 6991 companies. For more detailed information, please visit ECHA C&L website.* *Of the 67 notification(s) provided by 6989 of 6991 companies with hazard statement code(s).* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

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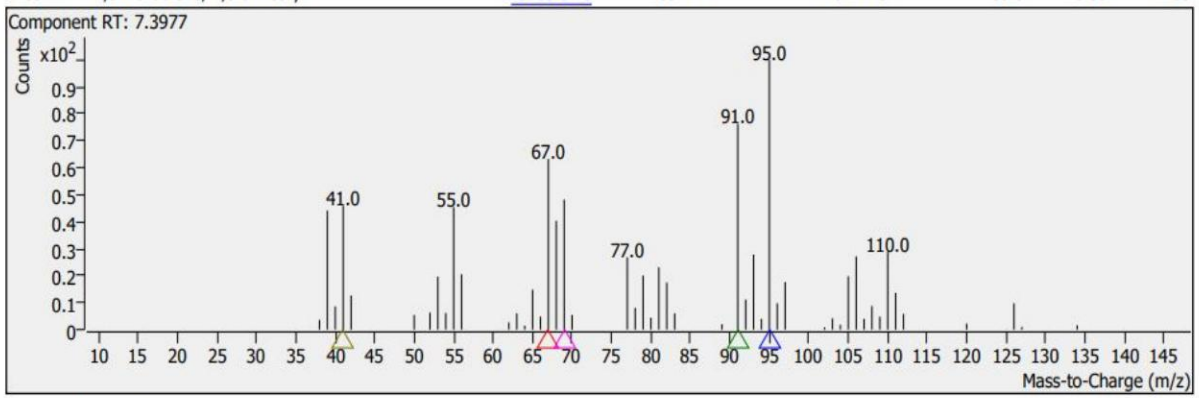
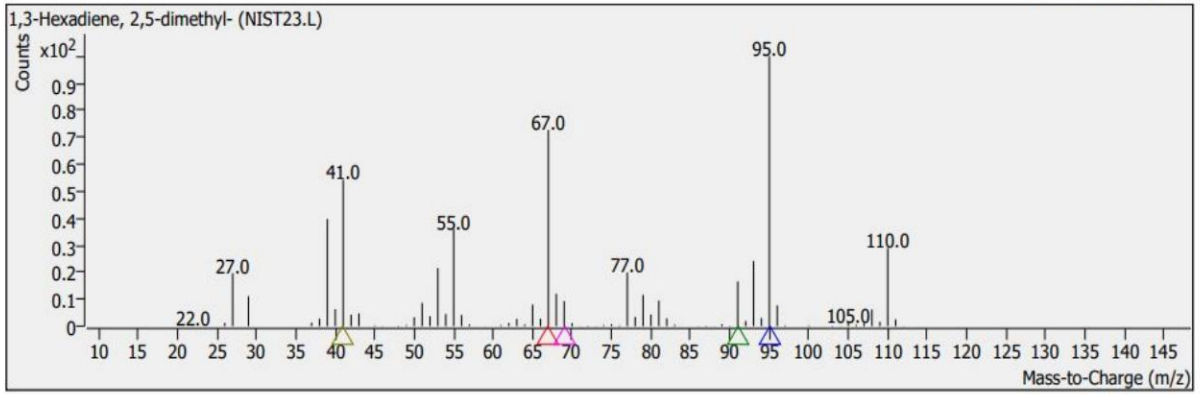
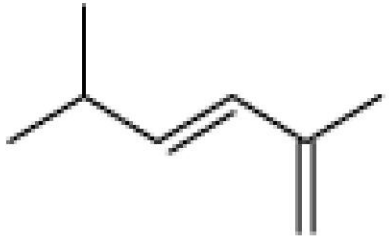
1,3-Hexadien, 2,5-dimethyl-, CAS 29253-64-3 / RT = 7,3977 [ÿ 0,9 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
7.3977	1,3-Hexadiene, 2,5-dimethyl-	29253-64-3	C8H14	14077119		83.6	0.85	2.83







2. Hazard identification

2.1 Classification of the substance or mixture

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s)	no data available
Signal word	no data available
Hazard statement(s)	no data available
Precautionary statement(s)	
Prevention	no data available
Response	no data available
Storage	no data available
Disposal	no data available

?

2.3 Other hazards which do not result in classification

no data available

3. Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
2,5-dimethylhexa-1,3-diene	2,5-dimethylhexa-1,3-diene	29253-64-3	none	100%

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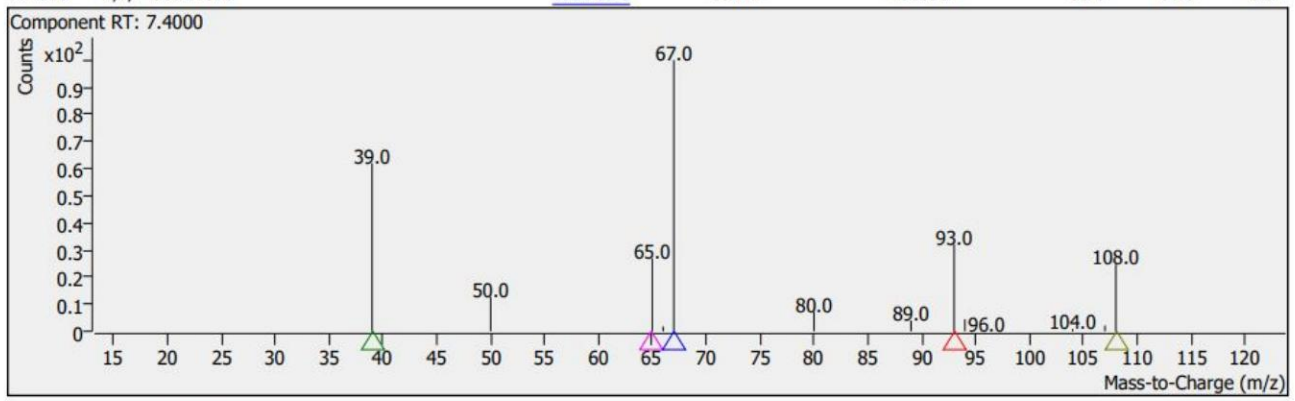
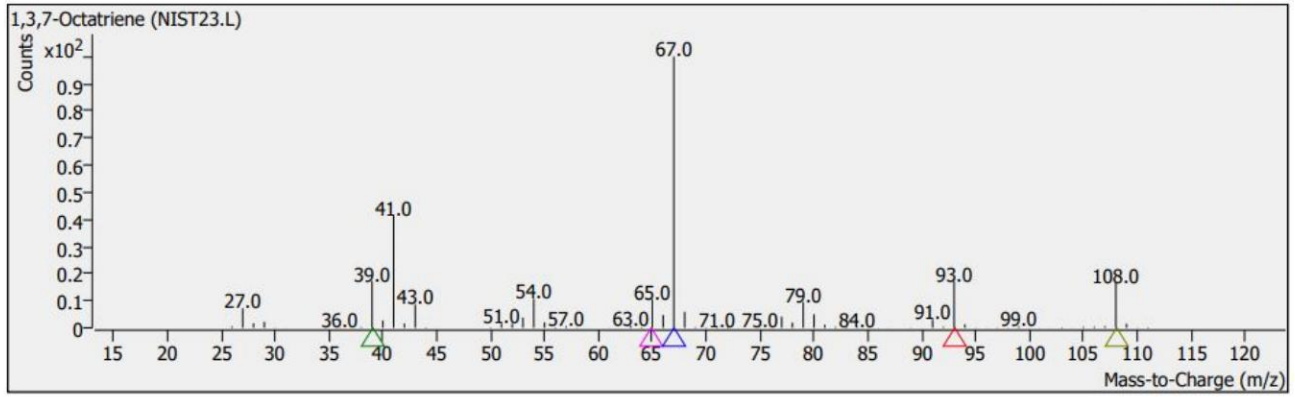
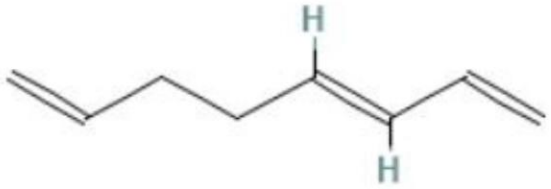
1,3,7-octatrien, CAS 1002-35-2 / RT = 7,4 [ÿ 0,3 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
7.4000	1,3,7-Octatriene	1002-35-3	C8H12	4836937		59.8	0.29	0.97







Safety Data

Back Directory

[Symbol(GHS)]

GHS02

[Signal word]

Danger

[Hazard statements]

H225

[Precautionary statements]

P210-P233-P240-P241-P242-P243-P280-P303+P361+P353-P370+P378-P403+P235-P501

Hazard Information

Back Directory

[Synthesis Reference(s)]

Journal of the American Chemical Society, 89, p. 6793, 1967 **DOI:** 10.1021/ja01001a089

Tags:1002-35-3 Related Product Information

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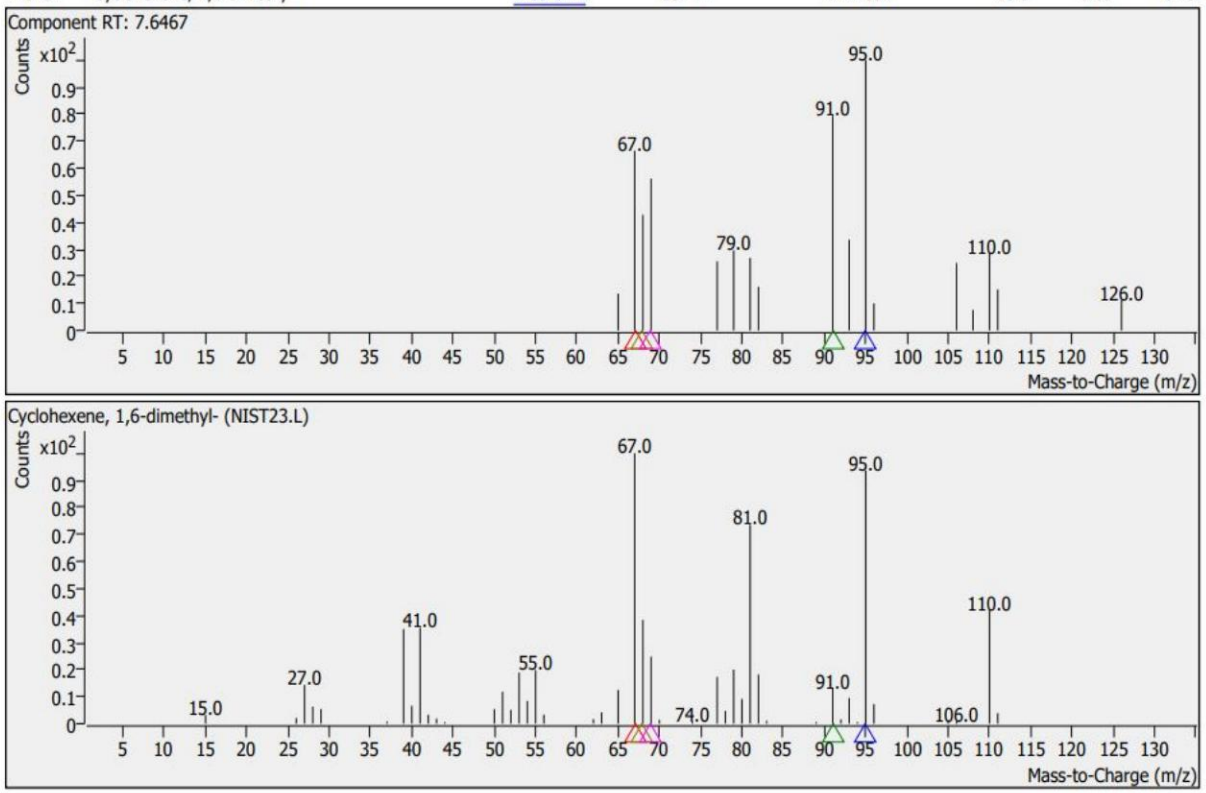
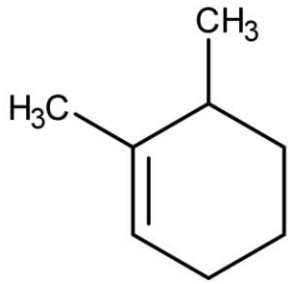
Cyclohexen, 1,6-dimethyl, CAS 1759-64-4 / RT = 7,6467 [ÿ 0,1 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
7.6467	Cyclohexene, 1,6-dimethyl-	1759-64-4	C8H14	1424397		68.5	0.09	0.29





2. Hazard identification

2.1 Classification of the substance or mixture

no data available

2.2 GHS label elements, including precautionary statements

Pictogram(s)	no data available
Signal word	no data available
Hazard statement(s)	no data available
Precautionary statement(s)	
Prevention	no data available
Response	no data available
Storage	no data available
Disposal	no data available

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2.3 Other hazards which do not result in classification

no data available

3. Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
1,6-DIMETHYLCYCLOHEXENE	1,6-DIMETHYLCYCLOHEXENE	1759-64-4	none	100%

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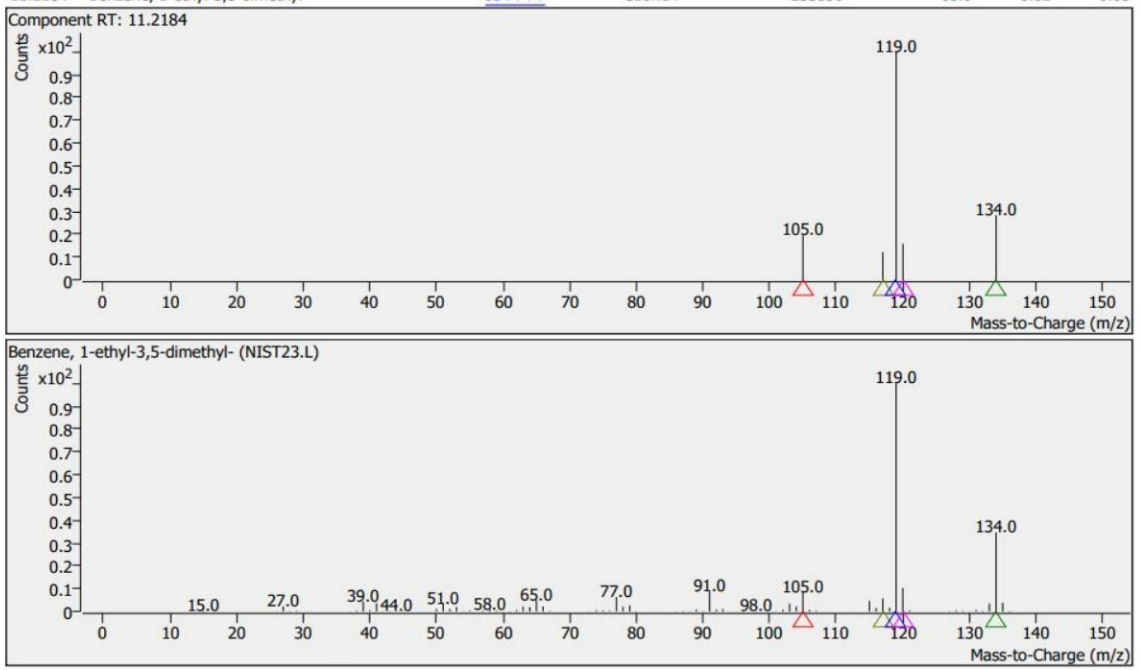
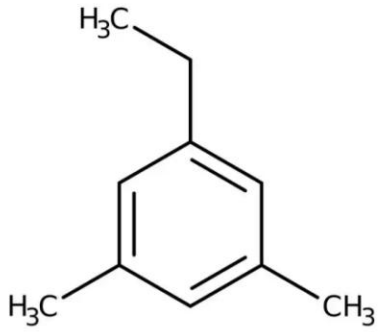
Benzen, 1-ethyl-3,5-dimethyl- / RT = 11,2184 [ÿ 0,02 areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
11.2184	Benzene, 1-ethyl-3,5-dimethyl-	934-74-7	C10H14	253850		68.0	0.02	0.05





1 GHS Classification

Pictogram(s)	Flammable, Irritant
Signal	Danger
GHS Hazard Statements	H225 (13.33%): Highly Flammable liquid and vapor [Danger Flammable liquids] H302 (84.44%): Harmful if swallowed [Warning Acute toxicity, oral] H317 (84.44%): May cause an allergic skin reaction [Warning Sensitization, Skin]
Precautionary Statement Codes	P210, P233, P240, P241, P242, P243, P261, P264, P270, P272, P280, P301+P317, P302+P352, P303+P361+P353, P321, P330, P333+P317, P362+P364, P370+P378, P403+P235, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 48 companies from 4 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 3 of 48 companies. For more detailed information, please visit ECHA C&L website.* *Of the 3 notification(s) provided by 45 of 48 companies with hazard statement code(s).* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

1-Ethyl-3,5-dimethylbenzene

PubChem CID	13627
Structure	2D, 3D
Chemical Safety	Flammable, Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{10}H_{14}$
Synonyms	1-Ethyl-3,5-dimethylbenzene 5-Ethyl-m-xylene 934-74-7 1,3-DIMETHYL-5-ETHYLBENZENE m-Xylene, 5-ethyl- View More...
Molecular Weight	134.22 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-03-26 Modify: 2024-05-11

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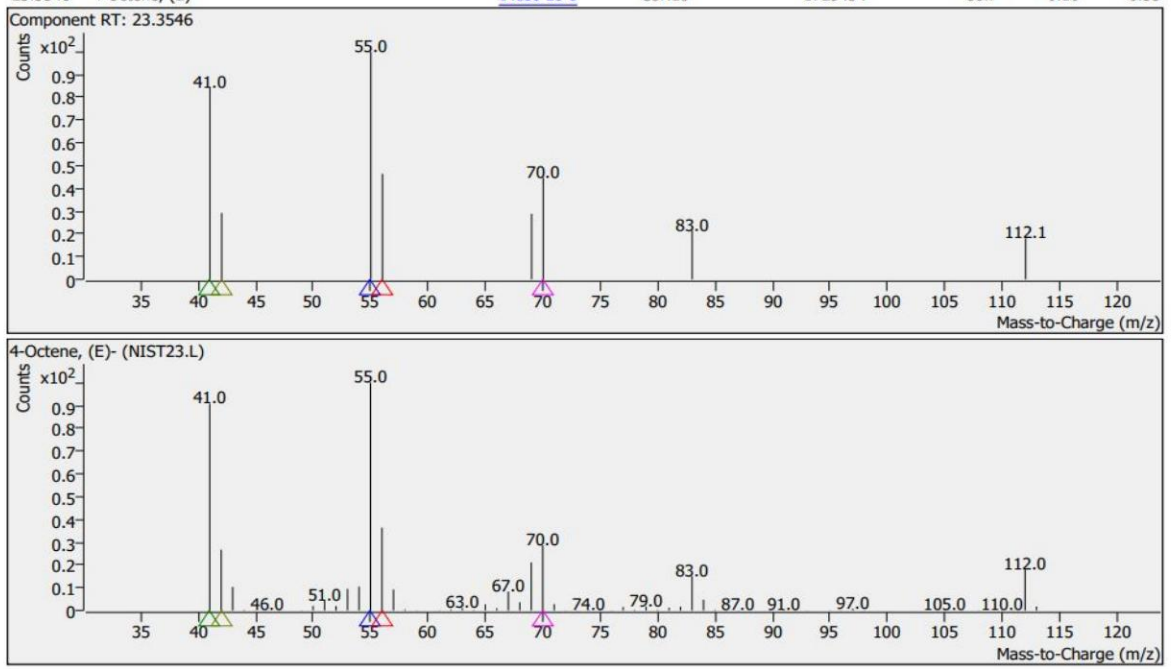
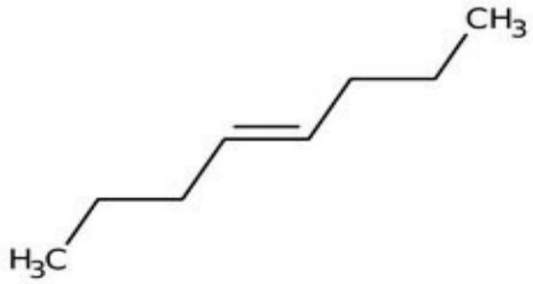
4-Octene, (E), CAS 14850-23-8 / RT = 23,3546 [ÿ 0,1 Areal%]

RT	Compound Name	CAS#	Formula	Area	MI	Match Score	Sample	Sample
23.3546	4-Octene, (E)-	14850-23-8	C8H16	1729434		80.7	0.10	0.35





2.2 GHS label elements, including precautionary statements

Pictogram(s)

Signal word	Danger
Hazard statement(s)	H225 Highly flammable liquid and vapour
	H304 May be fatal if swallowed and enters airways
Precautionary statement(s)	
Prevention	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
	P233 Keep container tightly closed.
	P240 Ground and bond container and receiving equipment.
	P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
	P242 Use non-sparking tools.
	P243 Take action to prevent static discharges.
	P280 Wear protective gloves/protective clothing/eye protection/face protection.
Response	P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].
	P370+P378 In case of fire: Use ... to extinguish.
	P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor/\u2026
	P331 Do NOT induce vomiting.
Storage	P403+P235 Store in a well-ventilated place. Keep cool.
	P405 Store locked up.
Disposal	P501 Dispose of contents/container to ...

2.3 Other hazards which do not result in classification

none

3. Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
TRANS-4-OCTENE	TRANS-4-OCTENE	14850-23-8	none	100%

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Kort opsummering af analysen

1. Fibrene består af polymerer baseret på adskillige naturlige aminosyrer syrer/derivater. De er bionedbrydelige.

2. Den gennemsnitlige fiberdiameter er et par µm og har indre hulrum, der indeholder materiale, dvs. kemiske stoffer. Efter opløsningsmiddelekstraktion kan der blandt disse stoffer detekteres kemiske forbindelser, som blandt andet er giftige, ætsende, sundhedsskadelige eller farlige for vand.

3. Patentet EP 1755382 B1 beskriver anvendelser, der gør det muligt at fylde fibrene med landbrugsmæssige (pesticider…) eller medicinske aktive ingredienser og lignende og at bruge dem til at målrette plante(dele) eller andre "biologiske systemer såsom lemmer (hænder, fødder, ben) hos mennesker eller dyr".

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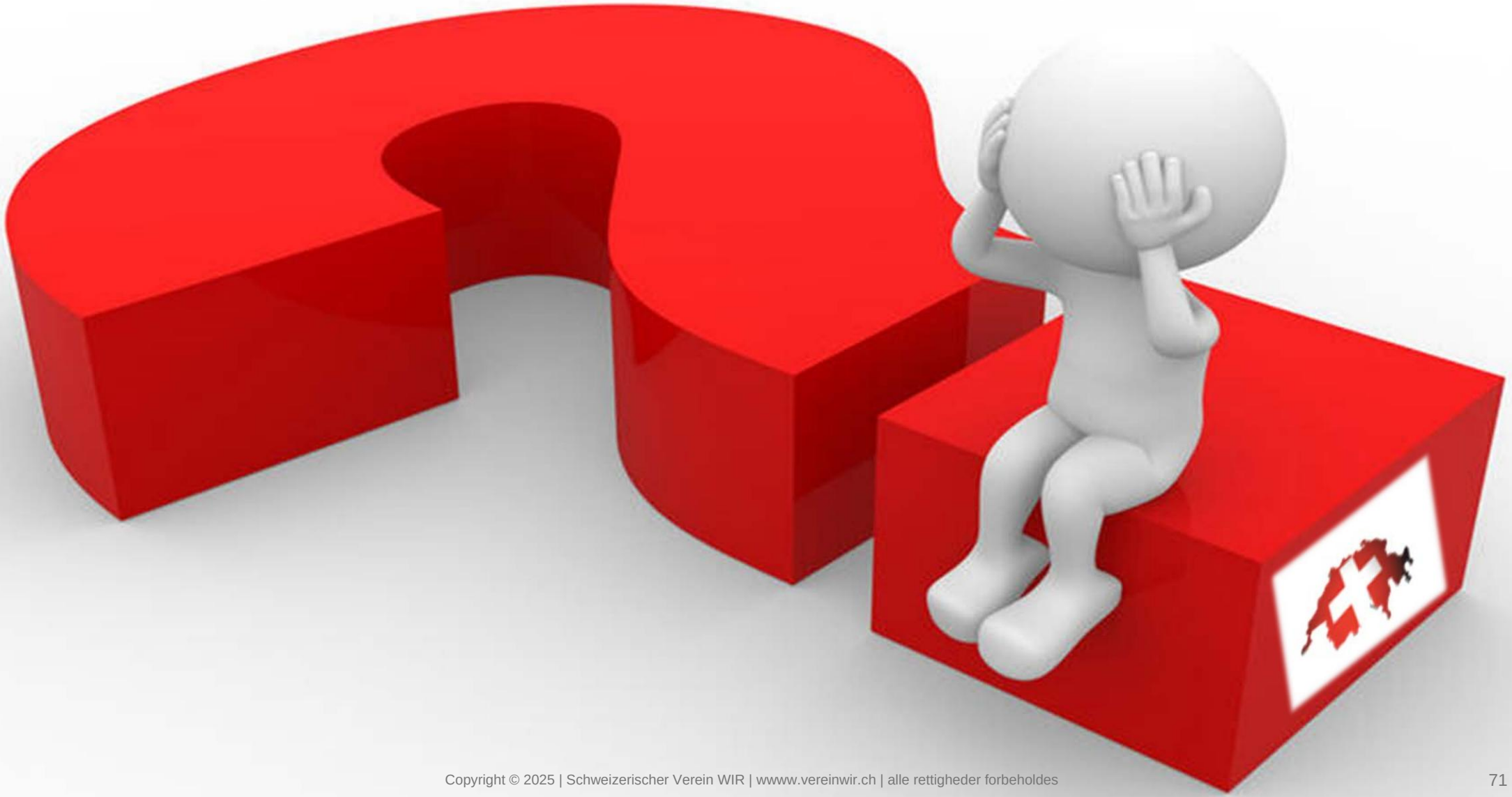
Spørgsmål og svar-session



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